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# **Semiclassical Quantization Via Adiabatic Switching**

## **Part I: Choice of Tori and Initial Conditions for Two-Dimensional Systems**

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**SEMICLASSICAL QUANTIZATION VIA ADIABATIC SWITCHING  
I.CHOICE OF TORI AND INITIAL CONDITIONS  
FOR TWO-DIMENSIONAL SYSTEMS**

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## Abstract

A general theoretical base and a general strategy for implementing semiclassical quantization using the adiabatic switching method is presented for two dimensional systems. The method proposed does not depend on specialized coordinates, trajectory or surfaces of section studies and is generalizable to many dimensional systems. The method gives quantum energies at a useful level of accuracy for the vast majority of states in many of the well known nonresonant and resonant Hamiltonian cases. Many eigenvalues previously thought unobtainable when using the adiabatic switching method are obtained in a quite simple manner.

## I. Introduction

Despite the recent development in computer technology which enabled very large scale quantum calculations of atomic and molecular energy levels the field of semiclassical (SC) quantization remains an extremely active area of research. The SC approach presents a tempting alternative to costly quantum calculations especially for multidimensional systems, where reliable quantum methods are still sometimes impossible to apply. Additionally, insights may be frequently gained using the SC methods, that lead to deeper understanding of the physics of complicated systems. This in turn may stimulate “classically guided” quantum approaches<sup>1</sup>.

During the last ten years a large number of different SC methods have been proposed. As a result, it is no longer possible to even briefly summarize the existing work in this field. Instead, we refer the reader to several, representative review articles<sup>2</sup> where a comparison of different SC methods is to be found.

Most of the SC methods rely on the well known EBK quantization of phase space tori. A crucial problem with these approaches is that it is necessary to find the trajectories which satisfy the EBK quantization condition. This may become a very hard and numerically inefficient task for systems with more than two degrees of freedom. Therefore most of the recently proposed methods<sup>2</sup> aim to minimize the work in finding the EBK tori.

It is known that EBK based methods must fail when the corresponding classical motion is chaotic and no EBK tori exist. On the other hand such methods as algebraic SC quantization of high order classical perturbation theory expansions<sup>3,4</sup> and the so called adiabatic switching method (AS) are seemingly able to quantize trajectories in the mildly chaotic region of the phase space.

The aim of the present paper is to pursue further the development of the AS method of SC quantization. The method, based on the adiabatic invariance principle originally discussed by Ehrenfest<sup>5</sup>, has been proposed and numerically tested by Solov'ev<sup>6</sup> and independently by Johnson<sup>7</sup>. It has been applied with success to a number of examples from different areas of physics<sup>8-16</sup>. It has been used also to generate SC wavefunctions<sup>17</sup>, locate stable periodic orbits<sup>18</sup> and to study the famous standard map<sup>19</sup>. On the negative side, it has been frequently stressed that the method may be difficult to apply for strongly resonant systems<sup>20,21</sup>. In this paper we present an unambiguous way to find the *vast majority* of SC energy levels (in the regular and mildly chaotic regime) using the AS method.

In this paper we will concentrate on two-dimensional (2D) systems. Here, unlike systems with more degrees of freedom (see the following paper) we can be guided in switching by changes in topology of the tori and the trajectories<sup>10</sup> (for the description of the AS method see Sec.II) . While being aware of such changes, we will not incorporate this knowledge into our method. The reason is that we seek methods valid in higher dimensions where such topological information is difficult, if not presently impossible, to obtain. Hence, we use well known results of classical and quantum mechanics to properly formulate the initial conditions, and rely on the magnitude of standard deviations to serve as the basic test of the method's success . The examples in Section V will show that this can be done successfully.

The proposed method is **general**. Although we mainly discuss the important case of coupled harmonic oscillators (normal modes), the extension to other systems (like coupled Morse oscillators or rotors) is straightforward; we give a prescription for an arbitrary system. As in any generalization, the work presented benefits from earlier works on the AS method. Section II therefore gives a brief review of the method itself and a complete (we hope) synopsis of the work performed up to the present by different groups. In Section III a review of relevant topics from classical and quantum mechanics is given. The general approach we propose is outlined in Section IV, while exemplary results supporting our

analysis are presented in Section V. Finally conclusions, comparison with other SC methods and future perspectives are the content of Section VI. In the accompanying paper which follows this one, the generalization of the method to systems with more degrees of freedom is discussed and the results of SC quantizations of multidimensional realistic ( $\text{SO}_2$ ) as well as model systems are presented.

## II. The Adiabatic Switching Method

As mentioned in the Introduction most EBK based SC methods suffer from the difficulty of locating the “quantizable tori” i.e. tori whose actions satisfy the assumed quantization conditions. An elegant method of avoiding this problem has been proposed in the pioneering work of Solov’ev<sup>6</sup>. The method is based on an original remark due to Ehrenfest<sup>7</sup>, who suggested that the quantizable tori of the nonintegrable system may be obtained from the corresponding tori of the integrable system by adiabatic changes of the parameters characterizing the system.

The adiabatic invariance theorem has been established for one-dimensional (1D) systems. Discussion of it can be found in standard textbooks on classical mechanics<sup>22–24</sup>. In essence, it states that the action (or any function of it) of a bound 1D trajectory generated by a time-dependent Hamiltonian  $H(t)$  is conserved whenever the temporal variations of  $H(t)$  are small on a time scale large compared to the intrinsic time scale determined by the instantaneous frequency  $\omega(t)$ :

$$\frac{dH(t)}{dt} \ll H(t)\omega(t) \quad (1)$$

This implies that the action is not conserved (no matter how slow the changes of  $H(t)$  are) when the trajectory crosses a separatrix. In fact the non zero change of adiabatic invariant in this case may be approximated quantitatively<sup>25</sup>.

The adiabatic theorem may be generalized to separable systems<sup>23,24</sup>, but it obviously fails for nonintegrable systems which generically exhibit chaotic behavior. Several approximate approaches have been proposed (for a review see Ref.23,24). Physically one might suspect that adiabatic invariance is approximately preserved for near-integrable systems. This claim is supported by a number of successful implementations of the AS method<sup>6–19</sup>.

The practical realization of SC quantization utilizing the adiabatic invariance assumption (coined the adiabatic switching (AS) method) proceeds as follows. For a given classical Hamiltonian  $H = H(\mathbf{p}, \mathbf{q})$  a new time-dependent Hamilton function is constructed:

$$H_s(t) = H_0^r + \lambda(t/T)(H - H_0^r) \quad (2)$$

where  $\lambda(x)$  satisfies  $\lambda(0) = 0$ ,  $\lambda(1) = 1$ . As  $t$  changes between 0 and the switching time  $T$ ,  $H_s$  describes a continuous family of systems evolving from  $H_0^r$  to  $H$ .  $H_0^r$  is assumed simple enough (usually separable) to allow for its efficient SC quantization. The initial conditions at  $t = 0$  are chosen to lie on a “quantizable torus” of  $H_0^r$ . Then the equations of motion defined by the Hamiltonian  $H_s(t)$  are integrated up to the time  $T$ . One then appeals to Ehrenfest’s conjecture and hopes that (for sufficiently large  $T$ ) the final values lie on the “quantizable torus” of  $H$ , that is they also have quantized values of the actions. As  $H_s$  is time-dependent, the energy is not conserved during the switching. The final energy should reproduce the SC energy of  $H$  corresponding to the chosen quantized actions.

Note that the procedure outlined above does not require  $H - H_0^r$  to be small. Clearly, for a generic  $H$ , in view of possible chaotic motion and passage through separatrices during switching, this approach does not have to produce good results. Therefore a deep understanding of the dynamics of the system, as well as clear criteria to determine the validity of the obtained results are needed for practical quantitative applications.

Already in early application of the method<sup>6</sup> it was realized that the above prescription does not specify  $H_0^r$  and that by a choice of the most appropriate  $H_0^r$  one may optimize the obtained results. Also for a given  $H_0^r$ , the choice of action variables is frequently not unique and this may be used to advantage.

To start let us recall, that classical perturbation theory defines in a consistent way the approximate invariants for Hamiltonians of the form  $H = H_0 + \epsilon H_1$ ;  $\epsilon$  being a small parameter<sup>23,24</sup> (see Sec.IIIA). Solov’ev<sup>6</sup> used classical perturbation theory as a guide to choose the appropriate action variables from which to switch for a given  $H_0^r$ .

Solov'ev points out that a smooth change of trajectory caustics is an indication of the approximate conservation of the adiabatic invariants. Thus he suggests that the reference Hamiltonian  $H_0^r$  should be chosen to assure that quantized trajectories of the final  $H$  are similar in shape to that of  $H_0^r$ . He also suggested the use of an ensemble of trajectories and calculated the final energy as an average of energies of individual trajectories. The initial points were chosen according to a probability density given by the modulus squared of the SC wavefunction of  $H_0^r$ .

Johnson, not being aware of Solov'ev's work, independently proposed the AS method<sup>7</sup>. By studying different switching functions  $\lambda(t)$ , he finds the form which later became used in the majority of applications (it turns out, not surprizingly, that quality of results depends crucially on the smoothness of  $\lambda(t)$ ). He applied the method to model Hamiltonians, similar to those discussed by Solov'ev.

Instead of averaging Johnson utilized a Fourier transform (FT) analysis of final energies to pick initial conditions non-randomly so to minimize nonadiabatic effects. In Sec.V this method and our proposed modification will be discussed in detail.

The very important paper of Skodje et al.<sup>10</sup> presented a detailed analysis of the SC quantization via the AS method. The authors point out that the similarity of the caustics of the initial and the final trajectory is not sufficient as a test of the successful implementation of the method. They emphasize the importance of strong resonance zones encountered during the process of switching, an effect which Solov'ev<sup>6</sup> chose to ignore. On the other hand, Skodje et al. pointed out that weak high order resonances did not in general destroy the approximate adiabatic invariance. These authors were the first to notice that averaging final energies not only gave the approximate SC energy, but also could be used to compute the standard (root mean squared) deviation (SD) which in turn acts as a quantitative measure of the accuracy of the obtained results. Skodje et al. exemplify the importance of strong resonant zones in several examples, pointing out, that by appropriate choice of  $H_0^r$  or by splitting the "switched on" part,  $H - H_0^r$ , into several contribution to be

switched consecutively, one may succeed in avoiding the resonant zones and thereby obtain more reliable results. This method, which they termed the “resonance avoidance method” requires, however, considerable insight into the system dynamics. This in turn weights heavily on the application of the AS method in practical calculations. Detailed studies of the system dynamics are time-consuming and for multidimensional (i.e. more than two dimensional) systems are quite difficult to perform. Probably being aware of this difficulty, the authors applied their method numerically<sup>10</sup> only to systems in which the resonant zones encountered at the beginning of the switching could be avoided.

An interesting contribution by Patterson<sup>12</sup> addressed the SC quantization of mildly chaotic classical systems using the AS method (Skodje et al<sup>10</sup> had noticed that AS apparently properly quantized some chaotic trajectories in the sense of obtaining good energies and reasonable SD's). Utilizing a quantum-mechanical viewpoint, Patterson looked for the influence of avoided crossings on the results. He found that the the AS method is capable of “overcoming” sharp avoided crossings (manifestations of secondary resonance zones) provided that they were passed through diabatically. This finding correlates with discovery of Skodje et al. that the energies of states obtained by quantizing trajectories in mildly chaotic regions can be optimized by the appropriate adjustment of the switching time  $T$  which is chosen so as to minimize the corresponding SD's.

Important modifications to the AS method were introduced by Grozdanov et al<sup>13,14</sup>. The appropriate choice of  $H_0^r$  in a treatment of the Henon-Heiles system enabled these authors to obtain excellent results for the so called “librator” states. A novel modification was introduced at the level of the choice of initial conditions. Instead of using the probability distribution determined by the SC wavefunction or the uniform sampling of the appropriate, but rarely known for a given  $H_0^r$ , angle variables, Grozdanov et al<sup>13</sup> randomly sampled the coordinates. For each choice of coordinates the initial momenta were determined from the expressions relating the actions to the  $\mathbf{p}, \mathbf{q}$  and into which quantized values of the actions were substituted. This strictly speaking, “informal” procedure is

justified in Sec.IV. The advantage of this method is evident in that it enormously enlarges the possible choice of  $H_0^r$ .

In the treatment of the 2 : 1, Fermi resonant system another important generalization was proposed<sup>14</sup>. It was known<sup>26</sup> that the Hamiltonian of two uncoupled harmonic oscillators with a 2 : 1 frequency ratio was separable in parabolic coordinates. For the particular coupling term in the model coupled oscillators Hamiltonian, the parabolic separation constant  $K$  is proportional to the first order classical perturbation theory correction to the unperturbed motion.  $K$  is therefore a first order adiabatic invariant of  $H$ . This suggests that this coordinate system is well adapted to this particular perturbation. Nevertheless, although the action variables may be formally expressed in terms of the integrals over appropriate parabolic coordinates, their direct quantization still requires considerable effort. The authors obtained the set of equations defining the torus by equating the quantum eigenvalues of  $K$  and  $H_0^r$  to their classical expressions in terms of  $\mathbf{p}, \mathbf{q}$ . To find points on the torus these equations were solved for the  $\mathbf{p}$ 's for each choice of  $\mathbf{q}$ 's ("informal method"). Again, very good results were obtained. Moreover, as pointed out by the authors elsewhere<sup>27</sup>, taking the quantum value of  $K$  (instead of the SC one resulting from the action quantization) effectively accounts for the quantum effects of tunneling and over barrier reflection present in the reference Hamiltonian  $H_0^r = H_0^h + \alpha K$ ; i.e. the method is semiclassically uniform in low order.

Recently, Saini and Farrelly<sup>16</sup> applied the AS method to the hydrogen atom in a strong magnetic field. In the chosen coordinate system (cylindrical coordinates) the pure hydrogen Hamiltonian is not separable. The authors, however, extended to this case the "informal" method for choosing the initial conditions. They also, following Grozdanov et al<sup>14</sup>, used quantum values of the first order adiabatic invariant to locate the initial torus.

As shown in this short review section, the AS method has undergone a quite rapid development. The interest in the method lies in its apparent simplicity, effectiveness and easy numerical implementation. There are still, however, important unanswered questions.

First is, how to prescribe a unified, general method for making the best choice of the  $H_0^r$  and the quantization conditions? How to deal with strongly resonant systems? Do we really need to study intensively the topology of the perturbed Hamiltonian (as has been done in all of the mentioned applications)? The main objections to the AS method<sup>20,21</sup> come from the ambiguity and general vagueness of the answers to these questions.

In this paper we seek to resolve these remaining problems. We claim that the approach proposed in Sec.IV and exemplified in Sec.V leads to a method which allows for “blind switching” i.e. the reasonable application of the AS method to a rich variety of Hamiltonians without a detailed study of trajectory shapes, tori déformations, caustics etc.

As the proposed method relies heavily on known results from classical and quantum mechanics, in an effort to make the paper self explanatory, the related essential definitions and concepts are reviewed in the next section.

### III. The dynamics of two dimensional near-integrable systems

In this section we present a condensed review of classical and quantum properties of 2D systems. We concentrate mainly on the resonant systems, as here lies the clue to the general implementation of the AS method. The background presented in this section is necessary for understanding the ideas and techniques presented later. The experienced reader can proceed directly to Section IV where the concepts presented here are rather extensively used.

The section is divided into two separate subsections on classical and quantum systems, respectively. Understanding of both is a prerequisite for the successful application of the SC ideas which link these two viewpoints.

#### IIIA. Classical dynamics<sup>23,24</sup>.

Consider the general, two-dimensional Hamiltonian expressed in terms of action-angle variables  $(I_i, \Theta_i)$ :

$$H(I_1, I_2, \Theta_1, \Theta_2) = H_0(I_1, I_2) + \epsilon H_1(I_1, I_2, \Theta_1, \Theta_2). \quad (3)$$

Our aim is to find the best possible actions to characterize the motion governed by the Hamiltonian (3). The perturbation  $H_1$  may be expressed as a Fourier series in the angle variables:

$$H_1 = \sum_{l,m} H_{lm}(I_1, I_2) \exp\{i[l\Theta_1 + m\Theta_2]\}, \quad (3a)$$

Assume that the zero order frequencies,  $\omega_i^0(\mathbf{I}) = \partial H_0(\mathbf{I})/\partial I_i$ , are in resonance (commensurate) i.e.  $\omega_1^0/\omega_2^0 = s/r$  for some values  $I_i^r$  of the actions. Standard perturbation theory usually then leads to the “small denominator” problem and secular perturbation theory must be used to remove the divergencies. Note that at the resonance  $\Theta_r = r\Theta_1 - s\Theta_2$  is an additional exact (local) constant of the motion of  $H_0$ . For small nonzero  $\epsilon$ ,  $\Theta_r$  varies slowly; its variation being a measure of the system’s deviation from the resonance. Thus  $\Theta_r$  constitutes the ideal slowly varying variable for adiabatic analysis. On the other hand the choice of the fast variable is ambiguous. The canonical transformation which identifies the slowly varying variable may be defined by its  $F_2$  generating function. Due to the freedom of choice of the fast variable any generating function of the form

$$F_2(\tilde{\mathbf{I}}, \boldsymbol{\Theta}) = A(r\Theta_1 - s\Theta_2)\tilde{I}_1 + f(\Theta_1, \Theta_2, \tilde{I}_2),$$

where  $A, f(\dots)$  are an arbitrary constant and arbitrary function, respectively, will serve our purpose. Let us make the following convenient choice:

$$F_2 = (2rs)^{-1}\{(r\Theta_1 - s\Theta_2)\tilde{I}_1 + (r\Theta_1 + s\Theta_2)\tilde{I}_2\} \quad (4),$$

leading to

$$\tilde{\Theta}_1 = (2rs)^{-1}(r\Theta_1 - s\Theta_2) = (2rs)^{-1}\Theta_r, \quad (5a)$$

$$\tilde{\Theta}_2 = (2rs)^{-1}(r\Theta_1 + s\Theta_2), \quad (5b)$$

$$\tilde{I}_1 = sI_1 - rI_2, \quad (5c)$$

$$\tilde{I}_2 = sI_1 + rI_2. \quad (5d)$$

The Fourier expansion (3a) expressed in the new, “tilded” variables is

$$\sum_{l,m} H_{lm}(\tilde{\mathbf{I}}) \exp\{i[(ls - mr)\tilde{\Theta}_1 + (ls + mr)\tilde{\Theta}_2]\}. \quad (6)$$

The average over the fast variable  $\tilde{\Theta}_2$  leaves only the terms satisfying  $ls + mr = 0$ :

$$\bar{H}_1(\tilde{I}_1, \tilde{\Theta}_1) = \sum_{p=-\infty}^{\infty} H_{(-pr, ps)}(\tilde{\mathbf{I}}) \exp\{-2i(rs)p\tilde{\Theta}_1\}. \quad (7)$$

The averaging is valid when  $\frac{d\tilde{\Theta}_1}{dt} \ll \frac{d\tilde{\Theta}_2}{dt}$  i.e. only near the resonance. The averaged Hamiltonian

$$\bar{H} = H_0(\tilde{I}_1, \tilde{I}_2) + \epsilon \bar{H}_1(\tilde{I}_1, \tilde{I}_2, \tilde{\Theta}_1)$$

is by construction independent of, i.e. cyclic in,  $\tilde{\Theta}_2$ ; thus  $\tilde{I}_2$  is a proper (first order, valid for small  $\epsilon$  only) adiabatic invariant.  $\bar{H}$  is an effective, one-dimensional, thus integrable, Hamiltonian (in  $(\tilde{I}_1, \tilde{\Theta}_1)$  variables). As such a formal solution of the dynamics allows it to be expressed in terms of a single action (with  $\tilde{I}_2$  being the parameter)  $J_\epsilon$  i.e.  $\bar{H} = \bar{H}(\tilde{I}_2, J_\epsilon)$ . Note that by construction  $J_\epsilon$  is formally dependent on  $\epsilon$ . Recall, however, that the adiabatic theorem is valid for one-dimensional systems (see Sec II). If we change  $\epsilon$  slowly, the action  $J_\epsilon$  *will not* change. This proves that  $J_\epsilon$  is not dependent on  $\epsilon$  and we can drop the subscript denoting it simply as  $J$ . The set of two actions  $\tilde{I}_2, J$  is a unique set of actions that are conserved when  $H_0$  is perturbed by  $\epsilon H_1$ ,  $\epsilon$  being small.

The above procedure used to find these actions is a form of lowest order classical perturbation theory. Any other form, e.g. Birkhof-Gustavson normal form, produces in the lowest order results that are completely determined by  $\tilde{I}_2$  and  $J$ . As such these results are also adiabatic invariants. Our AS strategy will in an essential step equate these classical adiabatic invariants to quantum ones (Eqs.(16),(17),(18) below). As such, our method is based on switching from tori possessing quantized classical adiabatic invariants.

Further insight may be gained by additional approximations. Frequently Fourier components in (7) decrease rapidly as  $p$  increases. Leaving only the leading  $p = 0, \pm 1$  terms one obtains

$$\bar{H} = H_0(\tilde{\mathbf{I}}) + \epsilon H_{00}(\tilde{\mathbf{I}}) + 2\epsilon H_{-r,s}(\tilde{\mathbf{I}}) \cos(2rs)\tilde{\Theta}_1,$$

or coming back to the original action-angle variables

$$H = H_0(\mathbf{I}) + \epsilon H_{00}(\mathbf{I}) + 2\epsilon H_{-r,s}(\mathbf{I}) \cos(r\Theta_1 - s\Theta_2) \quad (8)$$

i.e. the well known resonance Hamiltonian with the so called “secular term”, which is dependent on the explicitly present  $\Theta_\mu$ .

There are two possible cases discussed in the literature<sup>23</sup>: accidental and intrinsic degeneracy. We discuss briefly their definitions and physical meaning for use in the following sections.

(a). Accidental degeneracy occurs when the resonance condition is satisfied only for particular values of actions  $I_1, I_2$ . This implies that  $H_0$  is nonlinear in at least one of these actions. The unperturbed Hamiltonian  $H_0$ , transformed to the “rotating, tilded coordinates” (5) is then a function of both new actions  $\tilde{I}_1$  and  $\tilde{I}_2$ . In this case the perturbation cannot induce large changes in the action  $\tilde{I}_1$  (which together with its conjugate variable  $\tilde{\Theta}_1$  describes the “slow” motion) as  $H_0$  strongly detunes from resonance when  $\tilde{I}_1$  changes. One can then expand the resonance Hamiltonian (8) around the value of  $\tilde{I}_1$  corresponding to the center of the resonance and neglect higher than quadratic terms. This leads to an effective Hamiltonian isomorphic to that of the pendulum<sup>23,28</sup>. The effective motion may be either of the librating or of the rotating type which are separated by the separatrix. For future applications, let us point out, that although  $J$  (see above) is the conserved (to the lowest order) action, the error made assuming  $\tilde{I}_1$  is conserved is relatively small.

(b). Intrinsic degeneracy occurs when the resonance condition is satisfied for all values of  $I_1, I_2$ .  $\tilde{\Theta}_1$  is then a global constant of the unperturbed motion and  $H_0$  is a function of  $\tilde{I}_2$  only:  $H_0 = H_0(\tilde{I}_2) = H_0(rI_1 + sI_2)$ . The popular example of the intrinsic degeneracy is the case of two uncoupled harmonic oscillators with commensurate frequencies. Contrary to the accidental degeneracy case, large changes in  $\tilde{I}_1$  are possible as  $H_0$  is  $\tilde{I}_1$  independent. Similar expansion as in the previous case is not possible as changes of  $\tilde{I}_1, \tilde{\Theta}_1$  are of the same order. Instead one can make separate expansions around elliptic fixed points of  $(\tilde{I}_1, \tilde{\Theta}_1)$  motion<sup>23</sup>. Around each of them, this procedure leads to an effective harmonic oscillator Hamiltonian and to librating type motion. The different librating motions (centered around different fixed points) are separated by the separatrix. The separatrix separates also the resonant zones from the nonresonant zone. The volume of the phase space occupied by the resonant zones is large as compared to that in the accidental degeneracy case (compare

Fig.2.8 of Ref.23).

It happens frequently, especially for model, high symmetry Hamiltonians, that the above first order terms vanish. One has then to carry the secular perturbation theory to higher order. A similar distinction between intrinsic and accidental degeneracy still holds as it is determined by the  $H_0$ . The important case to be distinguished is however when in the first nonvanishing order only an angle-independent  $H_{00}$  term appears and secular terms are of higher order. Then it is justified to include the  $H_{00}$  term in the “modified”  $H_0^{mod}$ . The new “zero” order Hamiltonian depends now on both actions,  $H_0^{mod} = H_0 + \epsilon H_{00} \equiv H_0^{mod}(\tilde{I}_1, \tilde{I}_2)$ , where  $j=1,2$  depending on the lowest order in which  $H_{00}$  term appears. The “modified” representation gives a near degenerate (if  $H_{00}$  lifts the degeneracy) system. In this case, the degeneracy of the Hamiltonian will rather be of accidental, not intrinsic character.

Finally for larger  $\epsilon$  secondary resonance zones appear, which strictly speaking destroy the  $\tilde{I}_2, J$  adiabatic invariants. In the generic case, however, secondary resonance zones are much smaller in size than the primary ones. It has been pointed out<sup>23</sup> that the rapid reduction in size of higher-order resonance zones (islands) suggest that the lowest order invariants persist in the neighborhood of the primary fixed points. For still higher couplings as the resonance zones start to overlap<sup>28</sup>, chaotic motion, previously restricted to thin stochastic layers surrounding the separatrixes becomes important.

To end this subsection let us briefly concentrate on the specific case of coupled harmonic oscillators. The Hamiltonian is:

$$H = \frac{1}{2} \{ p_1^2 + p_2^2 + \omega_1^2 q_1^2 + \omega_2^2 q_2^2 \} + \sum_{k,l \geq 2} \alpha_{k,l} q_1^k q_2^l \quad (9)$$

with  $\omega_1 = r\omega$ ,  $\omega_2 = s\omega$ ;  $r,s$  - integers (for simplicity of discussion we neglect kinetic-type couplings of the form  $p_1^m p_2^n$ ). The obvious choice of  $H_0$  is the uncoupled system. The resonance condition is then fulfilled for all  $I_1, I_2$  i.e. the system is, by definition, intrinsically degenerate. Usually the sum in (9) is finite in practical applications, the

power of monomials  $q_1^k q_2^l$  being limited to some power  $M$  ( $k + l \leq M$ ). The lowest power term leading to secular behaviour (in the first order) is  $q_1^s q_2^r$ . For relatively large  $r, s$  the model Hamiltonians discussed in the literature frequently do not contain this term (due to limitation on  $M$ ). This is the case for the extensively studied<sup>20,29-31</sup> 3 : 4 resonance Hamiltonian (see Sec.V). As pointed out above the distinction between intrinsic and accidental degeneracy is in such cases ambiguous (see also the discussion in Ref.20).

### III B. Quantum mechanics

As in the classical case we concentrate mainly on zero order degenerate systems. Contrary to the previous subsection we begin our discussion with the particular, important case of coupled harmonic oscillators. In this case the formalism may be nicely represented in terms of creation and annihilation operators. The generalization to other systems is straightforward.

The Hamiltonian we are considering is the quantum version of (9) with  $q_i, p_i$  now being operators:

$$H = \frac{1}{2} \{p_1^2 + p_2^2 + \omega_1^2 q_1^2 + \omega_2^2 q_2^2\} + \epsilon \sum_{k,l \geq 2} \alpha_{k,l} q_1^k q_2^l. \quad (10)$$

Introducing the creation and annihilation operators:

$$a = 2^{-1/2} \{ \omega_1^{1/2} q_1 + i \omega_1^{-1/2} p_1 \}$$

$$a^+ = 2^{-1/2} \{ \omega_1^{1/2} q_1 - i \omega_1^{-1/2} p_1 \}$$

$$b = 2^{-1/2} \{ \omega_2^{1/2} q_2 + i \omega_2^{-1/2} p_2 \}$$

$$b^+ = 2^{-1/2} \{ \omega_2^{1/2} q_2 - i \omega_2^{-1/2} p_2 \}$$

the Hamiltonian (10) takes the form:

$$H = \omega_1(a^\dagger a + \frac{1}{2}) + \omega_2(b^\dagger b + \frac{1}{2}) + \epsilon \sum_{k,l=2}^{\infty} \frac{\alpha_{k,l}}{(2\omega_1)^{k/2}(2\omega_2)^{l/2}} (a^\dagger + a)^k (b^\dagger + b)^l \quad (11)$$

Assume as in the classical case that the frequencies are commensurate i.e.  $\omega_1/\omega_2 = s\omega/r\omega$ .

The uncoupled oscillators “zero order” Hamiltonian becomes

$$H_0 = \omega[s(a^\dagger a + \frac{1}{2}) + r(b^\dagger b + \frac{1}{2})] \quad (12)$$

The symmetry of  $H_0$  has been extensively discussed in the literature<sup>21,32,33</sup>. Its high symmetry results in a large set of observables commuting with (12). Any mutually commuting pair of these observables completely characterizes the spectrum of  $H_0$ . The one obvious choice is  $A \equiv H_0/\omega$  which describes the total excitation of the unperturbed system. Different eigenvalues  $N$  of  $A$  correspond to different degenerate manifolds. There is a finite number of low lying nondegenerate states; for them  $N < rs$ . A second observable is needed to differentiate between states within the manifold. The simplest possible operators that do not change  $N$  are  $a^\dagger a$ ,  $b^\dagger b$ ,  $(a^\dagger)^r b^s$  and  $a^r (b^\dagger)^s$ . The last two are non-hermitian and we have to construct observables out of them. The simplest choice is:

$$K \equiv (a^\dagger)^r b^s + a^r (b^\dagger)^s, \quad (13a)$$

$$L \equiv i[(a^\dagger)^r b^s - a^r (b^\dagger)^s]. \quad (13b)$$

The operators  $a^\dagger a$ ,  $b^\dagger b$  are occupation operators of individual modes. As we have already fixed  $A$  which is a weighted sum of them, it is natural to choose their weighted difference:

$$M \equiv sa^\dagger a - rb^\dagger b \quad (13c)$$

as a symmetrized combination.

The operators  $K, L, M$  do not commute with each other; all three of them by construction commute with  $A$ . The operators (13) turn out to be deeply related to the SU(2) symmetry of  $H_0$  that is shared with the corresponding classical system<sup>21,32,33</sup>.

Obviously  $K, L, M$  are not the only possible choices for the second (the first is  $A$ ) observable. In general any analytic function of  $A, K, L, M$  and the identity operator can be used as a second, commuting with  $A$  observable. It's choice should be determined by the nature of the perturbation  $H - H_0$ . Before making our choice let us first qualitatively discuss the influence of the perturbation on the system.

In Fig.1 the level correlation diagram of the exemplary degenerate oscillator system is presented. For a very small perturbation the levels shift linearly with  $\epsilon$  when the first order contribution does not vanish or with  $\epsilon^2$  when the second order contribution is the first nonvanishing one. The different  $N$  manifolds are well separated;  $N$  is a good quantum number. The second quantum number which characterizes the states within the manifold may be simply defined by energy ordering; i.e. the lowest state has its value say  $N_1$  equal to 1, for the second one  $N_1 = 2$  up to the uppermost level in the manifold. This region of  $\epsilon$  will be referred to as a non- $N$  mixing region. The first nonvanishing order quantum perturbation theory works well until the levels in the correlation diagram begin to bend. That usually happens just before the appearance of the first avoided crossing between levels of different manifolds. Again this is the generic behaviour of the system. For some particular systems the levels may strongly bend before the manifolds start to overlap and even cross within the same manifold. When the uppermost states of one manifold begin to cross (in the adiabatic approximation) or rather undergo avoided crossings with lowest states of the neighboring manifold the inter- $N$  mixing region sets in. These first avoided crossings are usually sharp and narrow due to the fact that properties of the levels involved are drastically different (as easily seen from their very different directionality in the correlation diagram). This is frequently related to a different spacial localization of the corresponding wavefunctions. Note that for very small intervals of  $\epsilon$  at the crossing the states strongly mix and the original quantum numbers are no longer good ones. On the other hand as the splitting between levels is small, their energies are still, with small error, well approximated by the adiabatic values. For higher  $\epsilon$  the exact levels follow

their original, low  $\epsilon$  directionality; their wavefunctions are very close (in the overlap sense) to that for low  $\epsilon$ . All these properties are easily seen considering a two-level coupled model. Therefore the levels “*after*” the sharp avoided crossing are still well described by the original quantum numbers.

For still higher  $\epsilon$  (or higher excitation) less extreme, in the directionality sense, states begin to cross. Their avoided crossings are less sharp and wider in energy avoidance, leading to larger range of  $\epsilon$  values for which the states are strongly mixed. As  $\epsilon$  is increased further anticrossings occur one after the other, forbidding the states to “recover” their original quantum numbers in the wake of the anticrossing. The two state model description becomes insufficient to describe the individual wavefunctions and more and more “configurations” need to be taken into account. Finally (for sufficiently high energy or large  $\epsilon$ ) the region of multiple avoided crossings is reached which is an indication of irregular wavefunctions. The presented qualitative picture is a known<sup>34</sup> route to “quantum chaos” via the picture of avoided crossings.

From the above qualitative discussion it is clear that the best simple second observable which may be used to assign quantum numbers (at least for moderate energies or small  $\epsilon$ ) should be determined in principle from the perturbation expansion of the coupled part of the Hamiltonian matrix. Any other assignment will not be as good as already in the low-coupling perturbative limit the corresponding second quantum number is not even approximately conserved. This does not mean, however, that the SC quantization based on the “wrong”, *second* quantum number choice will produce entirely wrong result. As pointed out by Skodje et al<sup>10</sup> (and seen also from the qualitative picture given above) in the non- $N$  mixing region the energy is often primarily dependent on  $N$  (i.e. the principal quantum number, associated with the  $A$  operator) and only weakly on the second quantum number.

It is important to realize that the arguments and qualitative picture presented above are to a very large extent valid for arbitrary degenerate zero-order Hamiltonians which are

not necessarily in the form (11). One may always in principle define an operator (equivalent to  $A$ ) whose eigenvalues distinguish between different manifolds and a commuting second operator  $T$  which differentiates different states in the given manifold.

For future application in Section IV we need a practical prescription to find the eigenvalues of the  $T$  operator. Define the projection operator onto the  $N$  manifold  $P_N = \sum_{n_1} |N, n_1\rangle\langle N, n_1|$ , where  $n_1$  denotes an intra-manifold unperturbed eigenfunction index. Also define the complementary operator  $Q_N = 1 - P_N$ . Write the Hamiltonian in the shorthand notation  $H = H_0 + \epsilon V$ . Define the Green's function of the total system  $G(E) = (E - H)^{-1}$  and the zero-order Green's function  $G_0(E) = (E - H_0)^{-1}$ . Repeated use of the known equality<sup>35</sup>  $G(E) = G_0(E) + \epsilon G_0(E) V G(E)$  for the Green's function  $P_N G(E) P_N$  leads to (we now drop the index  $N$  for convenience):

$$P G(E) P = (E - H_{eff})^{-1}, \quad (14)$$

where

$$H_{eff} = P H_0 P + \epsilon P V P + \epsilon^2 P V Q \frac{1}{E - H_0} Q V P + \dots \quad (15)$$

For each manifold this procedure leads to a small matrix of the order of the manifold degeneracy, which then may be diagonalized.

Note that we need to use (15) in the lowest nonvanishing order only. Thus we may write  $H_{eff}$  in the form

$$H_{eff} = P H_0 P + \epsilon^j T, \quad (15a)$$

where  $j = 1$  when the first order term ( $P V P$ ) does not vanish and  $j = 2$  otherwise, and  $T$  is the desired operator. Diagonalization of  $H_{eff}$  gives the first nonvanishing order energies and also via (15a) the eigenvalues of the  $T$  operator. It can be written in spectral form in terms of its eigenvalues and the eigenfunctions of  $H_{eff}$ .

For the Hamiltonian (11) (or any other expressible in terms of annihilation/creation operators) further progress may be made by noting that the projections in (15) leave only

those combinations of  $a, a^+, b, b^+$  in the effective perturbation which preserve the quantum number  $N$ , thus  $[A, H_{eff}] = 0$ . Therefore  $H_{eff}$  and also  $T$  may be expressed in terms of  $A$ , the identity operator  $I$ , and the operators  $K, L, M$  defined by (13). Simply put, in a first [second] order example,  $V [VQ(E - H_0)^{-1}QV]$  is expressed in terms of creation and annihilation operators using eq.(10); then terms which do not preserve  $N$  are dropped. By using the commutation rules the result can be expressed as a function of  $A, I, K, L$  and  $M$ . Obtained in this way an analytic expression for  $H_{eff}$  (which is independent of the particular  $N$  manifold) speeds up the practical implementation of finding the eigenvalues of  $H_{eff}$  as matrix elements of combinations of creation/annihilation operators are easily evaluated. The analytic expression for the  $T$  operator allows for its direct association with its classical counterpart in the SC quantization applications presented in the next section.

#### IV. Adiabatic switching. The general strategy

In this section an unambiguous method is formulated for choosing initial quantizable tori and initial conditions (points on these tori) to be used in AS quantization of an arbitrary Hamiltonian. In the next section the numerical applications are given which exemplify the use of the method.

Our approach is a continuation of the line suggested (and applied to a very particular case) by Grozdanov et al<sup>13,14</sup>, with however important modifications and generalizations. First we discuss the method for the particular Hamiltonian (10) in detail (with possible straightforward generalization to “kinetic” couplings) as the case of coupled harmonic oscillators is very important in applications. At the end of the section we discuss the generalization to other systems. From now on quantum operators will be denoted by a “hat”  $\hat{\phantom{x}}$  wherever ambiguity between classical and quantum quantities could appear.

The discussion of the energy level behavior in the preceding section indicates that for a quite large range of the perturbation parameter  $\epsilon$  (in the formal expression for the Hamiltonian  $\hat{H} = \hat{H}_0 + \epsilon\hat{V}$ ) the levels can be followed up in  $\epsilon$  on the correlation diagram in the unique way. This extends beyond the lowest order quantum perturbation theory (straight line) region into the region of sharp avoided crossings (and exact crossings if any). Some “extreme” states may be even followed up to the region of “multiple avoided crossings”. This strongly suggests that as the reference Hamiltonian we can take the uncoupled harmonic oscillators Hamiltonian  $H_0^r = H_0^h$  and switch on the perturbation provided great care is taken to choose the initial conditions “in harmony” with the perturbation. Recall that we denoted the quantum perturbation operator (defined in Sec.III B) as  $\hat{T}$ . By  $T$  we denote its classical counterpart obtained by appropriate (secular if necessary) classical

perturbation theory. The alternative approach to that just suggested above will be to choose as the reference Hamiltonian  $H_0^r = H_0^h + \epsilon^j T$ , where as before  $j$  denotes the order at which a first nonvanishing contribution to  $T$  is obtained. The latter approach seems slightly advantageous as in this case the reference Hamiltonian is “closer” to the final  $H$ . The latter method will therefore be suggested for numerical applications in most cases.

The simple prescription for locating initial conditions for the AS procedure, based on the above observation is as follows. We discuss separately the resonant, non resonant and near resonant cases.

#### A. The resonant $s : r$ case.

We list the proposed procedure in steps:

1. Calculate the first nonvanishing (first or second order) quantum invariant  $\hat{T}$  in the operator form using the effective Hamiltonian approach as described in IIIB.
2. Find its classical counterpart  $T$  using secular perturbation theory or the Birkhoff-Gustavson normal form<sup>36,23,24</sup> to the *same* order in  $\epsilon$ .
3. Diagonalize  $\hat{H}_0 + \epsilon^j \hat{T}$  in each manifold and find the eigenvalues of  $\hat{T}$ .
4. Define the initial torus by the equations

$$E_i = E_{class} = H_0^h(\mathbf{q}, \mathbf{p}) + \epsilon^j T(\mathbf{q}, \mathbf{p}) \quad (16a)$$

$$T_i = T(\mathbf{q}, \mathbf{p}). \quad (16b)$$

5. Initial conditions on the torus are chosen by the “informal” procedure, introduced in Sec.II. The positions  $q_1, q_2$  are randomly chosen in the classically allowed region (at energy  $E_i$ ) of the configuration space. Eqs.(16) determine the corresponding momenta (usually they must be found numerically). As Eqs.(16) are in general nonlinear one

may get multiple real solutions (then one of them is accepted) or complex solutions (note that (16b) may sometimes allow for no real solution for  $p_1, p_2$  for a given pair  $q_1, q_2$ ). In the latter case we choose randomly new positions and continue until real solutions are found.

6. Repeat step 5 as many times as required to get a set of different initial conditions.
7. For each initial condition perform the AS procedure, integrating the equations of motion for Hamiltonian

$$H(t) = H_0^r + \lambda(t/T)(\epsilon V - \epsilon^j T).$$

Note that (16) is equivalent to:

$$E_0 = H_0^h(\mathbf{q}, \mathbf{p}), \tag{17a}$$

$$T_i = T(\mathbf{q}, \mathbf{p}), \tag{17b}$$

where  $E_0$  is the energy of the given uncoupled manifold. Thus the same initial conditions could be used to switch the whole perturbation from  $H_0^r = H_0^h$ . This is physically understandable as the proper zero order wavefunctions (chosen according to the perturbation) are the same for  $\hat{H}_0^h$  and  $\hat{H}_0^h + \epsilon^j \hat{T}$ . As the tori of  $H_0^h$  are degenerate (due to the “super”-symmetry of  $H_0^h$  all trajectories are periodic) Eqs (17) determine a subset of periodic orbits (trajectories) which under the perturbation  $T$  evolve into a single torus. Sometimes, but not always,  $T$  may after some algebraic manipulations be expressed in terms of the “global action”  $\tilde{I}_2$  which is a proper adiabatic invariant (see Sec.II, Eq.(5d) and the following discussion) and a *single* second known, e.g.  $SU(2)$ , action<sup>21</sup> (this is the case for the Hénon-Heiles system - see the next Section). Then one may avoid the “informal” method and quantize the actions in the following way. As

$$\tilde{I}_2 = E_0/\omega, \tag{18a}$$

$$\tilde{I}_2 = s(n_1 + 1/2) + r(n_2 + 1/2) \tag{18b}$$

where  $n_1, n_2$  are integers such that (18a) is satisfied for a given manifold. The expression for  $T$  in terms of the actions gives the value of the second action using the *quantum* value  $T_i$ . The harmonic oscillator angle variables corresponding to these actions<sup>21</sup> may then be chosen randomly and a transformation to the original  $\mathbf{q}, \mathbf{p}$  carried out giving the required initial conditions. The advantage of this modification (which, let us stress, is possible in special simple cases only) is that the initial conditions are properly randomly sampled on the torus. On the other hand the reference Hamiltonian is “farther away” from the final  $H$  than in eq.(16). It is worthwhile to point out that action variables quantized in this way do not lie *exactly* on the EBK torus. Only for very high quantum numbers will this difference (i.e the difference between the eigenvalues of the quantum perturbation operator  $\hat{T}$  and the EBK quantized values of  $T$ ) disappear. For low or moderate quantum numbers a small difference analogous to the so called Langer correction in the WKB theory<sup>37</sup> and due to anharmonicities may appear. Also purely quantum effects such as over barrier reflection and tunneling, if present in  $\hat{H}_0^r + \epsilon^j \hat{T}$ , are taken into account in our method. Thus the use of quantum values for  $T$  as in (17) and (16) provides a low order uniform<sup>38</sup> quantization<sup>27</sup>.

## B. The non resonant case.

In spirit we proceed in exactly the same way as described in case A. The procedure can be considerably simplified due to the trivial observation that the appropriate  $P$  subspace may be safely chosen to be one-dimensional (i.e.  $P = |\psi_0\rangle\langle\psi_0|$ , where  $\psi_0$  is the initial state wavefunction). The first nonvanishing order quantum invariant is then expressible entirely in terms of  $a^\dagger a, b^\dagger b$  and the unity operators. The simplest approach, therefore, is to quantize directly the actions  $I_1, I_2$  in the standard way. Setting  $H_0^r = H_0^h$  one may then switch the total perturbation (as discussed above) choosing randomly the angle variables

$\Theta_1, \Theta_2$ .

One may be tempted to use an approach analogous to that described above for the resonant case and use the quantum eigenvalues of the  $\hat{T}$  to get non-EBK values of the actions. As EBK quantization gives perfect quantum eigenvalues for individual harmonic oscillators no Langer-type correction exists in this case. Therefore this modified approach will improve results only when big anharmonicities set in at low energies.

### C. The near resonant case.

We proceed in the similar way as in the resonant case. If the frequencies are  $\omega_1 = (s + \alpha)\omega, \omega_2 = r\omega$  where  $r, s$  are relative prime integers and  $\alpha$  is small we construct the  $P$  space (and build up the classical invariant) as for the  $s : r$  resonant Hamiltonian.

The procedure described in cases A to C enables us to perform AS quantization for an arbitrary Hamiltonian of the form (9).

We now offer the equally simple prescription for an arbitrary Hamiltonian, provided that the lowest nonvanishing order classical perturbation theory may be carried out analytically. Note that in the procedure described above the operator form of  $\hat{T}$  was never actually used (except for comparison with its classical counterpart  $T$ ). We used only its eigenvalues  $T_i$  to set up the initial conditions in Eq.(16b). These eigenvalues are simply obtained from (degenerate if necessary) quantum perturbation theory in the lowest nonvanishing order. Therefore if we write the classical Hamiltonian once again in the form

$$H = H_0 + \epsilon V \tag{19}$$

we are still able to find, using the “informal” method, the appropriate initial condition for AS procedure provided that

1. The quantum eigenvalues of  $\hat{H}_0$  are known.

2. The lowest nonvanishing order (first or at most second) quantum perturbation corrections to these eigenvalues can be effectively calculated
3. An analytical form of  $T$  can be found to the *same* order in  $\epsilon$ .

The procedure is exactly equivalent to that already described for the resonant IV.A case. Some additional remarks, explanations and warnings are in order. We do not claim that the method described above will work well for the energies of all the states in the regular and classically weakly chaotic regime. We do claim, however, that the method will work for the *vast majority* of states. As the AS method is very simple to implement numerically the proposed method allows us to obtain most of the states in a simple way. All the states in the low energy (small  $\epsilon$ ) range are usually obtained with excellent accuracy (see Sec.V). For the higher energy region (larger  $\epsilon$ ) a very few states may be inaccurate. These energies are characterized by relatively large standard deviations (SD) as compared to nearby states. We refer to these states as “hard” states.

Some of the “hard” states may correspond to strongly chaotic trajectories. The SC quantization of these states cannot be improved by any of the existing SC methods. On the other hand some “hard” states may correspond to classically regular motion. The relatively large SD’s obtained in such cases are the indication of tori topology changes during the switching (separatrix crossing) and the breakdown of the approximate adiabatic invariance. Recall, however, the generic energy level correlation diagram (see Fig.1 for the resonant  $H_0$ ) discussed in Sec.IIIb. As long as we are studying the region of energies corresponding to isolated or sharp avoided crossings, which may be tested numerically by producing the level correlation diagram during the switching, we believe and demonstrate that despite the large SD’s, the SC energies obtained are in reasonable agreement with “true” quantum values. In practice we find, (see Sec.V)), that the accuracy of the SC obtained results is only worse by roughly one significant figure as compared to the “best” states, i.e. those characterized by small SD’s. *For these cases we justify the accuracy of the AS energy level results by viewing the AS as a continuation procedure that approximates perturbation theory. Our results*

*support this view.* As long as the correlation diagram is “well behaved” and perturbation theory holds the AS method seems to give good energies (not actions or topologies). This is intuitively reasonable as we have already noted that classical perturbation theory is carried out as in Section IIIA by first finding the adiabatic invariants. The combination of classical and quantum perturbation theory used here (Eqs.(16,17,18)) and the AS yields a mutually supportive system of computation.

We note paranthetically and it will be shown below that some of the states for which we can observe the separatrix crossing in 2D give small SD’s and excellent energies. Here the separatrix is weak and the final trajectory topology is correct (see Fig.2). The states are not “hard” in our language. In this case our method gives good energies, topologies and acceptable albeit not optimal actions.

What does one do for those few “hard” states for which our method fails? Our answer is to give up on the AS method and use a more time consuming other SC methods. It is well to note that the literature has many examples of states which the AS method is not supposed to be able to get while we will show that it treats them succesfully.

As discussed, one of the reasons for the violation of approximate adiabatic invariance is the separatrix crossing. In trying to get the hard states of Hénon-Heiles system (starting from our general  $H_0^r$ ) we have devised a strategy that minimizes the error at the separatrix crossing. The method is explained in detail in the next section for the Hénon-Heiles system. Let us note here only, that this method is easily implemented and seems to significantly improve the SC energies obtained by the AS method for “hard” states. When it gives significant improvements it provides a well defined way to approach the “hard” states. The error minimalization method, contrary to the resonance avoidance method does not involve other quantization schemes; is a modification of the AS method, and is not too time consuming.

## V. Examples

In this section some numerical applications of the proposed AS method to model two dimensional systems are presented. First we present and explain our implementation of the method to a popular 3 : 4 resonant Hamiltonian. As a second example we briefly discuss the results obtained for Fermi resonant 2 : 1 and 1 : 2 Hamiltonians. Some selected states of the Hénon-Heiles 1 : 1 resonant system are also treated to further exemplify the proposed technique. Finally we study the case of a non-resonant model Hamiltonian.

### V.A. The 3 : 4 resonant system.

The Hamiltonian studied is

$$H = H_0 + \lambda V, \quad (20)$$

where

$$H_0 = \frac{1}{2} \left\{ p_x^2 + p_y^2 + \omega_x^2 x^2 + \omega_y^2 y^2 \right\}, \quad (20a)$$

$$V = x^2 y \quad (20b)$$

and the chosen values of parameters are  $\omega_x = \sqrt{0.9}$ ,  $\omega_y = \sqrt{1.6}$  and  $\lambda = -0.08$ . This model system was originally studied by Sorbie and Handy<sup>29</sup> and later by Stratt et al.<sup>30</sup> in their investigation of nodal patterns of quantum eigenstates. The same system was considered by De Leon et al.<sup>31</sup> in the study of the relation between classical resonance zones and quantum mechanics. Recently, Martens and Ezra<sup>20</sup> calculated the SC energies of the Hamiltonian (20) using the so called Fourier transform method. They confined their study to moderately low lying states. This was done because the method chosen requires long integration times to resolve higher lying states in the energy region where the density of states is large.

The classical dynamics of the system is well understood<sup>20,29-31</sup>. For the values of the parameters chosen the classical escape energy (dissociation energy)  $E_D = 25.33$ . The classical motion is predominantly regular up to energy<sup>31</sup>  $E_C = 22$  as seen by a study of Poincaré surfaces of section. Up to energy  $E_1 = 16$  the phase space can be divided into the 3 : 4 primary resonance zone and the non-resonant zone<sup>20,29</sup>; also near this energy very small secondary resonance zones appear. Around  $E_2 = 19$  the secondary resonance zones get big although they are still much smaller than the primary 3 : 4 resonance zone<sup>31</sup>.

Let us correlate this picture with classical secular perturbation theory and quantum perturbation theory as in Section III. The coupling term  $V$  is a monomial of much smaller order than required for the resonance to appear in a low order of the perturbation theory (the secular term would be e.g.  $x^4 y^3$  for the 3 : 4 resonance discussed). The first (in  $\lambda$ ) order term vanishes and the classical second order term may be immediately written down by noting that (20) belongs to the family of Hamiltonians discussed by Robnik<sup>3</sup>. Explicitly it takes a form:

$$V_2 = \frac{\lambda^2}{\omega_2^2 - 4\omega_1^2} \left\{ \frac{2}{\omega_1 \omega_2} I_1 I_2 + 2 \frac{\omega_1^2 - 3/8 \omega_2^2}{(\omega_1 \omega_2)^2} I_1^2 \right\} \quad (21)$$

where  $I_1, I_2$  are the action variables of  $x, y$  modes. Expressing  $V_2$  in terms of the tilded actions  $\tilde{I}_1, \tilde{I}_2$  introduced in Section IIIA (5) one notices that  $V_2$  is independent of the angle variables. Thus its Fourier analysis trivially gives only the “ $H_{00}$ ” term. In other words  $\tilde{I}_1, \tilde{I}_2$  are good actions up to the second order. Similarly Eq.(21), not being dependent on angles  $\Theta_i$ , shows that  $I_1, I_2$  are also good actions.

Hence the Hamiltonian (20) is a good example of the case, where although  $H_0$  (uncoupled harmonic oscillators) is formally intrinsically degenerate, the effective  $H_0^r = H_0 + V_2$  is accidentally near degenerate as the angle-dependent coupling appears in higher than lowest nonvanishing order. A similar conclusion has been reached by Martens and Ezra<sup>20</sup>.

The quantum perturbation approach is straightforward. Express the coupling  $V$  in

terms of the  $a, a^+, b, b^+$  operators (15):

$$\hat{V} = \frac{\lambda}{2\omega_1\sqrt{2\omega_2}}(a + a^+)(a + a^+)(b + b^+) \quad (22)$$

Choose the subspaces  $P_N$  as described in section IIIB i.e. for a given  $N$  choose states with quantum numbers  $n_x, n_y$  such that  $3n_x + 4n_y = N$ .

By inspection the first order term,  $P\hat{V}P$ , vanishes. The second order term can be easily evaluated, noting that only the “diagonal” contributions appear in this order i.e. there is no path via  $\hat{V}$  linking two different states of the same degenerate manifold. In other words, nondegenerate perturbation theory would have given the same result. Let us compare the so obtained operator

$$\hat{V}_2 = \frac{\lambda^2}{\omega_2^2 - 4\omega_1^2} \left\{ \frac{2}{\omega_1\omega_2} (a^+a + 1/2)(b^+b + 1/2) + 2 \frac{\omega_1^2 - 3/8\omega_2^2}{(\omega_1\omega_2)^2} (a^+a + 1/2)^2 - \frac{3}{16\omega_1^2} \right\} \quad (23)$$

to the corresponding classical expression (21). EBK quantization of (21) is obtained by substituting  $I_{1,2} = n_{x,y} + 1/2$ . As  $\hat{V}_2$  is diagonal in the  $x, y$  basis one can compare directly the eigenvalues of  $\hat{V}_2$  with the semiclassical expression for  $V_2$ . The difference appears as a constant term  $C = -\frac{3\lambda^2}{16\omega_1^2(\omega_2^2 - 4\omega_1^2)}$ . Following the discussion in Section III we could quantize  $\tilde{I}_1, \tilde{I}_2$  in a “non-EBK” way by assuming  $\tilde{I}_2 = 3(n_x + 1/2) + 4(n_y + 1/2)$  and obtaining  $\tilde{I}_1$  by setting (21a) to be equal to the corresponding eigenvalue of  $\hat{V}_2$ . Inverting relation (5) gives then non-EBK values of  $I_1, I_2$ . Note however that as  $I_1, I_2$  are Cartesian actions corresponding to uncoupled harmonic oscillators the correction to the EBK values is expected to be small (especially in view of high dissociation energy  $E_D$  of the system). Thus without loosing accuracy in any significant way we may quantize  $I_1, I_2$  according to standard EBK rules:  $I_i = n_i + 1/2$ . By performing both EBK and the above non-EBK quantization, we have checked that the results obtained are very close and well within the error induced by the finite sampling of the angle variables. Therefore in the Tables only the results obtained using the EBK quantization rule are listed.

The results are generated by the average of 25 trajectories. We have chosen the uncoupled harmonic oscillators Hamiltonian  $H_0$  (20a) as a reference Hamiltonian  $H_0^c = H_0$

and we have switched the total perturbation. The switching time was chosen to be  $T = 400$ . As discussed in Section IV this results in  $H_0^r$  being “further” from the total  $H$  than if we had chosen  $H_0^{r'} = H_0 + V_2$ . In the latter case we would have had to use the “informal” method of finding the initial conditions. By choosing  $H_0^r = H_0$  one easily finds the initial conditions for integration of the equations of motion in Cartesian coordinates by using the known relations of action-angle variables to the Cartesian  $q_i, p_i$ .

The results obtained are presented in Tables I-IV. Due to the relatively large number of bound states of the system (20), only selected states are given. In Table I moderately low lying, even states (up to  $E \approx 2/3 E_D$ ) are collected. For these states a detailed comparison of our results to that obtained by other SC methods may be made. Note the table shows that in this energy region different principal number  $N$  manifolds do not overlap. All SC energies obtained by us in this region are in excellent agreement with quantum eigenvalues, *regardless of the topology of the final torus*. To exemplify this result, we present in Fig.2 the final trajectories for some selected states. In Fig.2(a-b) two quantizable trajectories for states 45 and 57 (counting only the even states) are shown. They have the well known<sup>20,31</sup> “pretzel” shape, indicating that their tori lie inside the 3 : 4 primary resonance zone. This has been confirmed further by the Poincaré surface of section (SOS) plots for the trajectories - not shown to save space. In Fig.2(c-d) quantizable trajectories for states 53 and 49 are plotted. As revealed by SOS plots these trajectories correspond to the motion close to the separatrix separating the resonant and the nonresonant zones. The trajectory depicted in Fig.2(c) (state 53) is “just inside” the resonance zone; the one in Fig.2(d) (state 49) is “just outside”, in the nonresonant zone. Finally in Fig.2(e-f) quantizable trajectories for states 60,64 are shown. They have deformed rectangular caustics and indeed the corresponding tori lie deep in the nonresonant zone. Note that, for state 64, close inspection of the trajectory in Fig.2(f) (and the corresponding SOS) reveals that strictly speaking this trajectory lies in some high order secondary resonance zone. Despite the different topologies of the trajectories depicted in Fig.2 the SC energies obtained are

all in excellent agreement with the quantum values. State by state comparison reveals that the SC values obtained by the AS method, even for the “*wrong topology*” cases are in *better* agreement with quantum eigenvalues than Sorbie and Handy’s early results<sup>29</sup> or the Fourier transform method of SC quantization values<sup>20</sup>.

In Table II states around  $E = 19$  are given. In this energy region perturbed manifolds mix. Only states corresponding to low excitation in the  $x$ -mode and high in  $y$ -mode i.e. extreme states, enter the energy region corresponding to the adjacent manifold. This quantum mechanically corresponds to the “sharp” avoided crossings region. Here we notice an overall slight increase in the standard deviations (SD) values. Again most of the SC energies obtained are in excellent agreement with quantum values.

Some of the states have, as compared to neighboring states, quite large SD’s (states 80, 85, 87, 91, 92). One might suspect that these are the “wrong topology” cases, i.e. the corresponding tori lie in the primary 3 : 4 resonance zone. Indeed this is the case e.g. for 85 and 87 states, as shown by the wavefunctions plots<sup>31</sup>. These states are in our language the “hard states”. However, note, that the SC energies obtained for these “hard states” by the “primitive”, blind switching approach differ here from our results for states that do not change topology by at most 1 in the forth significant figure. There is no ambiguity in states assignment. This is, in our opinion, quite satisfactory and acceptable.

Table III gives results close and slightly above  $E = E_C$ , which, as mentioned above, corresponds to the onset energy for classically chaotic motion in a significant volume of the phase space. An overall increase in the SD’s may be noted with the exception of the “extreme motion” states. Still a majority of the SC energies are in the excellent agreement with the quantum values even in this region, where *different manifolds overlap appreciably* (see the second column of Table III). Where available, Sorbie and Handy’s results<sup>29</sup> are given, they are, however, much worse as compared to the present AS values. There are no Fourier transform method values available here; let us stress again that these would be extremely difficult to get in this high density of states region. Again, some large SD “hard

states” are to be noted (e.g. 113, 114, 118, 121, 126, 131, 132). These may be due to a wrong topology or to mild chaos present in this energy region.. Plots of wavefunctions<sup>31</sup> corresponding to 113, 114 states reveal, that indeed these states are influenced by the 3 : 4 primary resonant zone. The very close values of the SC energies obtained for the 131, 132 states, which belong to the same manifold, strongly suggest that those two states are strongly coupled by the 3 : 4 resonance. Only for these two, out of the 25 consecutive states listed, are the AS values unacceptable.

Finally, in Table IV states close to the escape energy  $E_D$ , in classically predominantly chaotic region of energy are given for both even and odd parities. Overall order of magnitude increase in the SD’s is observed; with the notable favorable exception, again, for the “extreme” states. A similar decrease in the overall accuracy of the SC energies is to be noted. One expects that as the resonant zones “shrink” in size their influence becomes negligible and no special “hard state” treatment would improve the results. A possible exception to this statement are the “extreme” resonant states, located in the vicinity of the corresponding periodic orbit. SC results of comparable accuracy to ours may be obtained only by the method of algebraic quantization of very high order classical perturbation theory<sup>4</sup>. This latter method, however, suffers from an ambiguity in choosing an optimal quantization procedure (see Ref.4b, and also the discussion of the nonresonant Hamiltonian below).

To summarize the blind AS approach, i.e. suggested by low order perturbation theory, allows us to quantize with quite remarkable accuracy almost all “quasi-bound” states of Hamiltonian (20).

## V.B The Fermi resonance.

The model Hamiltonian is now

$$H = H_0 + \alpha x(y^2 + \beta x^2) \quad (24)$$

where  $H_0$  as before denotes the Hamiltonian of the uncoupled harmonic oscillators

$$H_0 = \frac{1}{2} \left\{ p_x^2 + p_y^2 + \omega_1^2 x^2 + \omega_2^2 y^2 \right\}$$

with  $\alpha = \beta = -0.08$  and two choices of zero order frequencies i.e.  $\omega_1 = 1.4, \omega_2 = 0.7$  (to be referred to as the 2 : 1 case) and  $\omega_1 = 0.7, \omega_2 = 1.4$  (the 1 : 2 case).

The 2 : 1 system has been discussed in detail by Grozdanov et al<sup>14</sup>. The implementation of the AS method used was a particular early application of the general approach introduced in this paper. Therefore, there is no need to reproduce these results once more. Let us summarize their findings in the language introduced here.

The perturbation,  $\alpha x(y^2 + \beta y^2)$  may be expressed in terms of the creation/annihilation operators:

$$\alpha \hat{V} = \frac{\alpha}{2\sqrt{2}\omega_1} \left\{ \frac{1}{\omega_2} (a + a^+)(b + b^+)(b + b^+) + \frac{\beta}{\omega_1} (a + a^+)(a + a^+)(a + a^+) \right\}. \quad (25)$$

Building the  $P$  subspaces corresponding to degenerate manifolds, and performing the quantum perturbation theory one finds easily that the first order term  $P\hat{V}P$  gives a nonvanishing contribution

$$\alpha P\hat{V}P = \frac{\alpha}{2\omega_2\sqrt{2}\omega_1} (a(b^+)^2 + a^+b^2) \equiv \hat{\alpha}\hat{K} \quad (25a)$$

where  $\hat{K} = a(b^+)^2 + a^+b^2$  is the resonant operator (see Sec.IIIB). Note that this is the only contribution in the first order, suggesting a strong resonant behaviour of the system. Corresponding classical perturbation theory leads to (see Ref.14 and references therein):

$$\alpha V_1 = \hat{\alpha} K, \quad (26)$$

with

$$K = 2 \left\{ 2\omega_1^{-1/2} y p_x p_y + \omega_1^{1/2} \omega_2 x y^2 + \omega_1^{1/2} \omega_2^{-1} x p_y^2 \right\}. \quad (26a)$$

The adiabatic averaging method (see Sec.IIIA, Eq.(5) and the following) shows that  $K$  gives a secular term; the following Fourier analysis produces no  $H_{00}$  term. This, again, shows that the phase space is dominated by the 2 : 1 resonance zone and the degeneracy is of the intrinsic type.

Indeed, the AS SC energies obtained by Grozdanov et al<sup>14</sup> using Eq.(16) were in excellent agreement with the exact quantum energies for all regular states of the system and in a very good agreement for states for which the quantizable trajectories lay close to the separatrix dividing the different topologies of the “up horseshoe” and the “down horseshoe” type. As seen from the discussion in Sec.IIIA, both up and down topologies are given by the different values of  $K$ . Large and small values of  $K$  correspond to the respective expansions about the two fixed points (see Sec.IIIA for a general discussion of intrinsic degeneracy and Ref.14 for more details on the AS quantization of this system).

Let us now turn our attention to the 1 : 2 case. Obviously, the degenerate manifolds here consist of different states than in 2 : 1 case discussed above. The  $xy^2$  term, which previously drove the resonance and gave a secular first order contribution now acts in a nonresonant way. As a result, the first order perturbation theory term vanishes. In the second order, apart from the diagonal terms (similar to that for 3 : 4 system) new terms appear that couple states within a degenerate manifold. These are of the form  $(a^+)^4 b^2$  and  $a^4 (b^+)^2$ . One might therefore expect the presence of a secular contribution in this order. It turns out, however, that these terms cancel out and the resulting expression is again purely diagonal in the  $x, y$  representation. One may therefore again expect that the majority of states will be properly quantized using the EBK actions of the individual oscillators. (Similar conclusions, based on the classical first order secular perturbation theory have been reached by Noid et al.<sup>26</sup>; here the validity of this conjecture is extended through the second order.)

In Table V some representative results for the AS quantization using Cartesian actions are tabulated for both even and odd states. As no comparison with other SC results is possible for highly excited states, and, as the system, as shown above, is similar to the 3 : 4 case discussed already in detail, we present only a few energy values. Again, not surprisingly, the overall agreement between the SC energies and the quantum eigenvalues is remarkably good for the majority of states. As the quantum diagonalizations were performed separately in the odd and even in  $y$  harmonic basis sets there is no possibility of level misassignment even for small splittings.

In analogy to the 3 : 4 case, few SC energies are obtained with worse than average accuracy. The corresponding trajectories probably lie in the 1 : 2 resonance zone; the corresponding SD's are relatively large as compared to other states. These “hard” states appear only for higher energies. Low lying states are without exception quantized accurately. This is due to the dominance of the lowest nonvanishing, nonresonant perturbation term in the low energy region<sup>10</sup>.

#### V.C The Hénon-Heiles, 1:1 resonant system.

The Hénon-Heiles (HH) system described by the Hamiltonian

$$H = \frac{1}{2} \left\{ p_x^2 + p_y^2 + x^2 + y^2 \right\} + \epsilon x(y^2 - x^2/3) \quad (27)$$

is probably the most often studied coupled oscillators problem. Here  $\epsilon = \sqrt{0.0125}$ . Numerous SC treatments for this system has been presented; a few of them using the AS method<sup>6,7,10,13</sup>. The Hamiltonian (27) is of high  $C_{3v}$  symmetry. As a result, the degeneracy of the uncoupled 1:1 resonant  $H_0$  is only partially lifted by the perturbation.

The classical studies revealed<sup>39</sup> that there are basically two types of trajectories of  $H$  in the regular regime, the so called precessors, with ring type topology, and librators with

a narrow box-like topology. It is interesting to investigate to what extent our “blind”, perturbation oriented method will be able to approximate the quantum eigenvalues for both types of states.

Let us briefly summarize the previous AS approaches to the problem (see also the discussion in Sec.II). Solov’ev’s<sup>6</sup> AS quantization was based on the classical perturbation theory; as such he switched the full perturbation from  $H_0^r = H_0$ , assuming that the angular momentum is an approximately good perturbed action variable. He claimed excellent agreement for his SC values with quantum energies, giving however, no numerical examples. Skodje et al.<sup>10</sup> similarly quantized the precessor states; for librators they used the unusual quantization scheme  $I_y = l/3, l = 0, 1, 2, \dots$  suggested by an early study of Noid and Marcus<sup>39</sup>. In the latter case they have chosen a different  $H_0^r$ , namely  $H_0^r = H_0 - 0.19x^2$ , in the spirit of their “resonance avoidance method”. Excellent agreement for the libration states was obtained in Ref.13, where the different choice,  $H_0^r = H_0 - \epsilon x^3/3$ , was made;  $I_y$  was quantized by the standard EBK rule and the “informal” method was used for the choice of the initial points on the  $H_0^r$  tori. Both of the above methods used several trajectories and averaged the final energies. Johnson<sup>7</sup>, for the same system, used a Fourier expansion in the angle variables to choose two trajectories for which leading nonadiabatic contributions to the final energies canceled out. He introduced the Langer-type correction for the angular momentum values and that greatly improved the accuracy for the lowest lying states.

Let us now proceed in the spirit of the general method of Sec.IV. The classical perturbation theory in the lowest nonvanishing order is quadratic in  $\epsilon$  and gives<sup>38,21a</sup>

$$V_2 = \frac{\epsilon^2}{12} (7L^2 - 5\tilde{I}_z^2) \quad (28)$$

showing that indeed the angular momentum  $L$  is a good approximate invariant (together with, as usual  $\tilde{I}_2 = I_1 + I_2 \equiv I_x + I_y$  (5)). The corresponding quantum perturbation theory in the operator form, after some algebraic manipulations gives the quantum perturbation

operator to second order in  $\epsilon$ :

$$\hat{V}_2 = \frac{\epsilon^2}{12}(7\hat{L}^2 - 5\hat{A}^2 + \frac{11}{3}) \quad (29)$$

where  $\hat{L} = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = i(ab^+ - ba^+)$  is the quantum angular momentum operator and  $\hat{A} = a^+a + b^+b + 1$  is the operator describing the total excitation (see Section IIIB). Note that both the classical  $V_2$  and the quantum  $\hat{V}_2$  quantities give identical results for  $\pm l$ , thus the corresponding degeneracy is not broken by the second order perturbation theory. Consideration of the  $C_{3v}$  symmetry of  $H$  reveals<sup>40</sup> that the appropriate basis set should be built up from symmetric and antisymmetric combinations of the  $|N, l\rangle$  states ( $N$  stands, as usual, for the principal quantum number). The quantum energy levels obtained show that, although most of the above remaining degeneracy is not lifted by the full  $H$ , eigenstates corresponding to  $l = \pm 3, j = 1, 2, \dots$  are split. This splitting appears in a higher order perturbative expansion and may be accounted for semiclassically in the uniform SC quantization of the Birkhoff-Gustavson<sup>36</sup> normal form<sup>4,38,41</sup>. Clearly, as there is no apparent way to build classical analogs of the linear combinations of  $|N, l\rangle$  states, the AS method cannot reproduce this splitting. As a result we can only compare the SC energies obtained for  $N, \pm l$  to the average of the two quantum energies.

To second order,  $L$ , together with the principal action  $I_2$  are good invariants. EBK quantization of  $\tilde{I}_2$  and  $L$  gives  $\tilde{I}_2 = N + 1$ ;  $N = 0, 1, 2, \dots$  and  $L = -N, -N + 2, \dots, N - 2, N$ . Note that such a quantization cannot give correct results for the lowest lying states as it neglects the constant term present in  $\hat{V}_2$ . Contrary to the 3 : 4 case discussed previously, this constant term is quantitatively important as will be shown below. To make the appropriate, non-EBK quantization we equate the eigenvalues of the second order Hamiltonian  $\hat{H}_2 \equiv \hat{A}_2 + \hat{V}_2$  with its classical counterpart  $H_2 = \tilde{I}_2 + V_2$

$$A + \frac{\epsilon^2}{12}(7l^2 - 5A^2 + 11/3) = \tilde{I}_2 + \frac{\epsilon^2}{12}(7L^2 - 5\tilde{I}_2^2), \quad (30)$$

where  $A$  stands for the eigenvalue of  $\hat{A}$ ;  $A = N + 1$ . As (30) should hold for arbitrary (in particular equal to 0)  $\epsilon$ , one immediately obtains the following quantization scheme:

$\tilde{I}_2 = N + 1$ ;  $N = 0, 1, \dots$  (as before) and  $L = \text{sgn}(l)\sqrt{l^2 + 11/21}$ , with  $l$  given by its quantum values  $l = -N, \dots, N - 2, N$ .

Note that this quantization scheme for the angular momentum is very close to the empirically obtained value of Johnson's Langer-type correction  $L = \text{sgn}(l)\sqrt{l^2 + 1/2}$ . The above derivation justifies Johnson's procedure. Obviously, for high  $l$ , the difference between the corrected (later referred to as the modified Langer correction) and the EBK value becomes negligible in accordance with the spirit of the SC theory.

Hence, according to the method of Section IV we define the quantized torus by the values of  $\tilde{I}_2$  and  $L$  given by the above quantization scheme (with the modified Langer correction). The initial points on the torus are determined by picking randomly the angle of rotation of the coordinate frame  $\gamma$  (this angle variable is conjugate to  $L$ ) and the sum of the initial phases of the individual oscillators  $\tilde{\Theta}_2$  (see Eq.(5)) as the variable conjugate to the  $\tilde{I}_2$ . Then we switch the full perturbation. As in the previously discussed cases, *the majority* of energies are obtained with great accuracy as compared to the quantum values. In Table VI results for some representative, "good topology" precessor states are collected. These are compared with earlier AS results of Johnson<sup>7</sup> and Skodje et al<sup>10</sup>. Note that the modified Langer correction leads to a great improvement for the lowest lying states; the agreement with the quantum values is extraordinary. On the other hand, as expected, the modified Langer correction becomes less important for highly excited states. Our results are in close agreement with those of Ref.10.

In Table VII the results (denoted as standard AS) for *all* "wrong topology" librator states are presented. The agreement with quantum values is worse, especially for moderately excited states. Note, however, that the majority of states of the HH system are of the precessor type; for them, "blind", perturbation theory guided AS works very well. The librators constitute the minority of "hard states".

Improvement for these "hard", low  $L$  states can be made without changing the reference Hamiltonian  $H_0^r$ . As the adiabatic invariance is destroyed during the passage through

the separatrix, it is not possible to get an improvement by adiabatically changing the Hamiltonian parameters. Is it possible, however, to pass through the separatrix diabatically? Such an approach was successful in treating small secondary resonance zones<sup>12</sup>. We tried, therefore, to decrease the switching time, hoping to minimize the SD's. The procedure did not work, probably because the nonadiabaticity introduced by the more rapid switching in other regions was stronger than the gain due to faster switching through the separatrix. At this point we were inspired by Johnson's<sup>7</sup> original method of minimizing the errors due to nonadiabaticity. He noticed, that individual final trajectories energies may be written as a Fourier series in the angle variables

$$E_i(T, \gamma, \tilde{\Theta}_2) = E_{av}(T) + \sum_{k,l} E_{k,l}(T) \exp\{i[k\gamma + l\tilde{\Theta}_2]\}. \quad (31)$$

By Fourier transforming a set of final energies corresponding to a single level, Johnson<sup>7</sup> has found that the dominant term is  $E_{6,0}$ . As noted in Ref.7 the Fourier analysis is not needed, this result can be inferred from the symmetry of the Hamiltonian (26). To minimize nonadiabatic effects, Johnson took two trajectories, with initial conditions differing by  $\gamma_0 = \pi/6$  and averaged the so obtained energies to cancel the contribution due to the  $E_{6,0}$  term in (31). All results reported in Ref.7 were obtained by averaging final energies of two trajectories started with the initial condition (in our notation)  $\tilde{\Theta}_2 = 0$ ,  $\gamma = 0$  and  $\tilde{\Theta}_2 = 0$ ,  $\gamma = \gamma_0$  and switched for relatively short times.

Note, however, that the procedure, just described, minimizes only the leading term in the Fourier expansion (31). Other terms in (31) may lead to errors as no additional average or special treatment of other terms was proposed<sup>7</sup>. We have found that by choosing different initial conditions (which still lead to minimizing the  $E_{6,0}$  term contribution) e.g.  $\tilde{\Theta}_2 = \alpha_1$ ,  $\gamma = \alpha_2$  and  $\tilde{\Theta}_2 = \alpha_1$ ,  $\gamma = \alpha_2 + \gamma_0$  ( $\alpha_1, \alpha_2$  arbitrary), that the results of Johnson's procedure strongly depend on the choice of  $\alpha_1$  and  $\alpha_2$ ; thus the agreement with the quantum eigenvalues obtained in Ref.7 is somewhat accidental (except for the low lying states).

It is important to realize that in order to minimize the influence of the other terms in (31) one may combine the Johnson's idea with a random average method. We propose the following procedure.

1. Choose randomly  $\tilde{\Theta}_2, \gamma$ .
2. Switch two trajectories started with the initial conditions  $\tilde{\Theta}_2, \gamma$  and  $\tilde{\Theta}_2, \gamma + \gamma_0$ .
3. Average the obtained two final energies to get the "pair averaged energy"  $E_i \equiv (E^1(\tilde{\Theta}_2, \gamma) + E^2(\tilde{\Theta}_2, \gamma + \gamma_0))/2$ .
4. Repeat steps 1 through 3 for an ensemble of trajectories (i.e. initial conditions  $\tilde{\Theta}_2, \gamma$ . Let  $n$  be the number of repeats.

One may then define the average energy

$$E = \frac{1}{n} \sum E_i \quad (32)$$

and the modified standard deviation (MSD):

$$MSD = \frac{1}{n} \sum (E_i - E)^2. \quad (33)$$

Note that MSD (33) differs from the typical SD as  $E_i$  in (33) are the "pair averaged energies" as defined in step 2 and not the individual final energies.

The "pair average" minimizes the influence of the leading term in (31); the subsequent average (32) takes care of the other terms. This procedure is, obviously, not needed for "good topology" states; numerous examples in this paper and previous AS attempts show that this is an unnecessary complication in these cases. For our present purpose, the described procedure is interesting. It assures that at least the leading term in (31) is almost exactly canceled and thus the effects of nonadiabacity due to the separatrix crossing as expressed by MSD will be greatly increased as compared to the typical SD.

With that in mind we have repeatedly switched the typical libration state (quantum numbers  $N = 8, l = 0$ ) for different switching times  $T$  looking for a minimum in the MSD. The MSD so obtained are shown as squares in Fig.3. The error bars correspond

to the difference in MSD's between the positive  $l$  and the negative  $l$  separate cases. For comparison the SD's are also shown as open circles in Fig.3. We have repeated this procedure for several libration-type states; the minimum generally appears around the  $T = 40$ . This value is an order of magnitude smaller than the typical switching time  $T = 400$  chosen for the “good topology” cases and incidentally is close to the  $T = 50$  value taken by Johnson<sup>7</sup>. Accepting  $T = 40$  we have switched all the libration states, the energies obtained according to (32) are also presented in Table VII. Also both the corresponding SD's and MSD's are shown there. The accuracy of the obtained results suggests that the procedure described should be also tried (with appropriate modifications) for other “wrong topology”, “hard” states of other systems.

Concluding this study of the Hénon-Heiles system let us stress, that due to proper, non-EBK quantization, we were able to obtain SC results in excellent agreement with the quantum values for the low lying states. “Wrong topology” librators' SC energies were improved over the standard AS approach with the help of the “modified Johnson procedure” using the same  $H_0^r$  as for the precessor states. The numbers speak for themselves.

#### V.D The nonresonant case.

Lastly, we present the results obtained for the nonresonant Hamiltonian of the form (24) with parameters  $\omega_1 = 0.7$ ,  $\omega_2 = 1.3$ ,  $\alpha = -0.1$ ,  $\beta = 0.1$ . The results of the AS method for this system have been already reported<sup>13</sup> but are superseded by the results presented here which are based on a larger sample of initial points and a smaller step size in the integration routine. As discussed in Sec.IV the approximately good Cartesian actions in the nonresonant case are the individual actions of uncoupled oscillators.

The results are collected in Table VIII, together with the results of the SC quantization of the Birkhoff-Gustavson normal form (BGNF) of Farrelly and Uzer<sup>4a</sup> and Fried and

Ezra<sup>4b</sup>. The first group of states lies in the moderately high energy region (about 3/4 of the classical escape energy  $E_D$ ). For these states the results of the SC quantization using the Fourier transform method are also available<sup>42</sup>. All quoted SC methods give the results of comparable accuracy in this energy region. Unquestionably, the AS method requires a much smaller amount of work that does the Fourier transform method or the 12<sup>th</sup> order BGNF with or without Pade resummation (the BGNF of this order may only be obtained numerically or using symbolic programming language). Notably the SC quantization of the 6<sup>th</sup> order BGNF gives results of much worse accuracy<sup>41</sup>.

Somewhat unexpectedly, similar conclusions hold for high lying states, in the vicinity of the dissociation energy  $E_D$ . Fortunately, due to other independent calculations<sup>4a,4b</sup>, we can compare our results with the results of the SC quantization of a 12<sup>th</sup> order BGNF, a 12<sup>th</sup> order BGNF with Pade resummation, a 16<sup>th</sup> order BGNF and the same form quantized according to the Weyl quantization rule (see Ref.4b for details). Two surprising observations may be made. The AS results are at least comparable in accuracy if not (for the 12 levels for which a comparison may be made) actually closer to the exact quantum values than the results of the SC quantization of the high order BGNF. Note also the unexpected large difference between the 12<sup>th</sup> order and the 16<sup>th</sup> order BGNF results indicating a breakdown of the perturbative approach. The Pade resummation results seem to be a bit closer to the exact quantum values than the straight SC quantization of the 12<sup>th</sup> order or the 16<sup>th</sup> order forms, still being, however, slightly inferior to the AS results. Weyl quantization of the BGNF seems to give comparable in accuracy results to that of the AS method, but as noted in Ref.4b, this approach produces less accurate results for lower lying states.

To summarize the results obtained for this nonresonant model system, the AS method gives at least as good SC energies as other sophisticated SC quantization schemes with, by far, much less effort involved in the calculation.

## VI. Conclusions

In this paper we have presented an unambiguous method for the choice of a proper tori and initial conditions to be used in the AS method. Our method is based on the quantum perturbation theory and as such assures excellent results for the low lying states. The discussion and a joint use of the classical and quantum ideas provides a basis for an empirically justified conjecture that the method works for most of the states whose classical analogs lie in the regular or weakly chaotic regions of the phase space. The perturbation theory based choice of tori assures that the correct, appropriate to the perturbation, topologies are generated for most of the states. The method is general and applicable whenever the lowest order classical perturbation theory may be carried out in the analytic way. In the frequently discussed coupled harmonic oscillators case, our approach is, therefore, entirely different than the one recently suggested<sup>21</sup> which puts emphasis on the  $SU(2)$  symmetry of the uncoupled problem.

The presented, perturbation guided, “blind” approach gives, as shown by several examples, good SC results even when during the switching of the full (not necessarily small) perturbation the adiabaticity is destroyed and the initial actions lost due e.g. to a separatrix crossing (and a corresponding change of the torus topology). In these cases we justify the use of the AS method by an analogy to the parameter dependence of the energy levels as shown by the level correlation diagram (see e.g. Fig.1). We expect the AS SC energies to approximate well quantum values up to the region of sharply avoided crossings or even sometimes in the region of isolated avoided crossings (see Sec.IIIB). In other words for energy values, which in quantum perturbation theory are always less sensitive to error than the wavefunctions or transition moments, our method works in most cases because the quantum perturbation theory (high order) still gives good results. For a relatively very few “hard states” (in the classically regular or mildly chaotic regions) our approach fails;

also it fails when the system is classically strongly chaotic, which roughly corresponds to the multiple “broad” avoided crossings part of the level correlation diagram.

The “hard states” which let us repeat constitute a small minority of states could be SC quantized either by choosing, in the spirit of the “resonance avoidance method”<sup>10</sup>, a different reference Hamiltonian  $H_0^r$  or by different, more time consuming SC methods.

In the original Solov’ev<sup>6</sup> paper an approach closely related to ours, but based purely on the EBK quantization of actions chosen according to classical perturbation theory, has been proposed. Our approach improves this proposition in two ways. First, by using quantum perturbation theory to properly choose the initial tori, we automatically overcome the possible problem with “Langer-type” corrections. Second, the use of the “informal” method makes the often difficult procedure of finding of action and angle variables unnecessary. This greatly simplifies the amount of work needed to implement the AS method.

The perturbation oriented approach, in the original formulation of Solov’ev, has been criticized by Skodje et al<sup>10</sup> as requiring a large pre-switching theoretical effort. They favored instead the “resonance avoidance method”. In our opinion the simplifications due to the “informal” method and the quality of results obtained using the quantum perturbation based AS method fully justify the moderate initial effort of calculating the lowest nonvanishing order of quantum and classical perturbation theory. The “resonance avoidance method” requires either a deep insight into the details of the system dynamics, making it much harder to use for multidimensional systems, or several guesses for different  $H_0^r$  which may greatly increase the amount of work needed to obtain good results. We rely on the standard deviation values and not topology studies to spot the possible topology changes. We generally accept the results as valid on the basis of the size of the SD and the obtained energy levels dependence on the switching parameter (i.e. SC level correlation diagram).

The successful quantization of 3 : 4 and 1:1 systems up to the classical escape energies gives convincing examples of the ability of the AS method to successfully quantize states

even when their classical analogs lie in the mildly chaotic regions of the phase space. This result<sup>10,12,14</sup> is a further justification of the procedure of following the classical (and quantum) correlation diagram as given above. It is quite generally accepted that the “quantum chaos” in the sense of irregular, patternless wavefunctions is “sluggish” in following the onset of the classically chaotic motion<sup>43</sup>. The results presented here support this idea.

Although the general approach has been presented here only for two degrees of freedom systems, its extension to higher dimensional systems is straightforward and is given in the following paper. As far as two dimensional systems are concerned, we intend to test the method further. We are completing the SC quantization of the Hydrogen atom in parallel magnetic and electric fields using the proposed method. The Edmonds-Pullen<sup>44</sup> 1:1 resonant Hamiltonian as well as a family of resonant model systems recently discussed by Noid and Marcus<sup>45</sup> should provide a stringent test of the method. All these systems are of the intrinsic degeneracy type with the secular term present, thus their treatment will be similar to the 2:1 Fermi resonant case. We intend also to perform the AS quantization of the near resonant 1:1 Barbanis Hamiltonian (see e.g. Ref.4). This system is quite similar to the H enon-Heiles system, the important difference being that no simple expression of the perturbation theory in terms of the angular momentum or any other known action is possible, thus the “informal” method for the choice of the initial points has to be used.

In our opinion, however, the numerical results presented here, fully justify our approach proposed in the present paper.

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### Figure captions

- Fig.1 Level correlation diagram for the Hydrogen atom in a strong magnetic field  $B$ . This system is equivalent to two coupled harmonic oscillators in a 1 : 1 intrinsic resonance. In a low  $B$  field limit the perturbation is proportional to  $B^2$  (the Zeeman linear shift is traditionally omitted). Note the straight line behavior of the levels as a function of  $B^2$  followed by sharp avoided crossings. Figure reproduced from Ref.46, courtesy of Dr. D. Wintgen.
- Fig.2 Final trajectories of the 3 : 4 resonant system obtained by the AS method for states 45(a), 57(b), 53(c), 49(d), 60(e) and 64(f). For further details see text.
- Fig.3 The behaviour of the MSD and the SD as a function of the switching time  $T$  for the  $|N, l\rangle = |8, 0\rangle$  state. Open squares correspond to the MSD (left hand scale). Note the deep minimum around  $T = 40$ . The error bars give the difference between two MSD's obtained for  $\pm l$  for a given  $T$ . Open circles give the usual SD's (right hand scale). For further details see text.

**TABLE I: States of 3:4 System**

State	N <sup>a</sup>	$n_x, n_y$ <sup>b</sup>	$E_{TC}$ <sup>c</sup>	$E_{FT}$ <sup>d</sup>	$E_{QM}$ <sup>e</sup>	$E_{AS}$ <sup>f</sup>	$SD$ <sup>g</sup>
45	42	10,3	–	13.9878	13.9822	13.9803	4.1(–3)
46	42	6,6	–	14.0605	14.0613	14.0606	3.4(–4)
47	42	14,0	–	14.0699	14.0723	14.0700	1.1(–4)
48	42	2,9	–	14.2451	14.2454	14.2454	1.4(–4)
49	44	12,2	–	14.5848 <sup>h</sup>	14.5845	14.5843	2.8(–3)
50	44	8,5	–	14.6072	14.6086	14.6072	1.7(–4)
51	44	4,8	–	14.7618	14.7624	14.7619	1.7(–4)
52	44	0,11	–	14.9901	14.9901	14.9900	0.9(–4)
53	46	10,4	15.1710	15.1705	15.1692	15.1684	3.7(–4)
54	46	14,1	15.2149	15.2152	15.2175	15.2154	7.4(–4)
55	46	6,7	15.2818	15.2827	15.2834	15.2829	3.6(–4)
56	46	2,10	15.4952	15.4957	15.4959	15.4961	0.8(–4)
57	48	12,3	15.7537	15.7582	15.7520	15.7478	8.7(–3)
58	48	8,6	15.8116	15.8121	15.8136	15.8129	7.6(–4)
59	48	16,0	15.8821	15.8825	15.8854	15.8826	1.3(–4)
60	48	4,9	15.9984	15.9989	15.9993	15.9992	1.3(–4)
61	48	0,12	15.2522	16.2523	16.2523	16.2523	1.1(–4)
62	50	10,5	16.3567	16.3429	16.3509	16.3566	6.8(–4)
63	50	14,2	16.3600	16.3617	16.3675	16.3621	2.3(–3)
64	50	6,8	16.5031	16.5043	16.5050	16.5047	3.5(–4)
65	50	2,11	16.7459	16.7462	16.7464	16.7465	1.1(–4)

a. Principal quantum number  $N = 3n_x + 4n_y$ .

b. Cartesian quantum numbers.

c. Trajectory closure method, SC results of Sorbie and Handy (ref. 29).

TABLE I: continued...

- d. Fourier transform method SC results of Martens and Ezra (ref. 20).
- e. Exact quantum mechanical results (1256 even in x, harmonic basis set).
- f. Present AS results, T=400 average of 25 trajectories.
- g. Standard deviations  $a(-b)$  stands for  $a \times 10^{-b}$ .
- h. The more favorable of the two numbers reported in ref. 20 is listed.

**TABLE II:** States of 3:4 System continued. Notation as in Table I.

State	N	$n_x, n_y$	$E_{TC}$	$E_{QM}$	$E_{AS}$	SD
80	58	14,4	-	18.6453	18.6908	2.1(-2)
81	58	10,7	-	18.7293	18.7280	1.3(-3)
82	56	0,14	-	18.7767	18.7768	<0.1(-4)
83	58	18,1	-	18.7799	18.7770	1.0(-3)
84	58	6,10	18.9448	18.9464	18.9467	3.4(-4)
85	60	16,3	-	19.2252	19.2399	1.3(-2)
86	58	2,13	-	19.2469	19.2469	0.5(-4)
87	60	12,6	-	19.2639	19.2552	2.1(-3)
88	60	8,9	-	19.4243	19.4236	6.6(-4)
89	60	20,0	19.4832	19.4838	19.4789	3.0(-4)
90	60	4,12	-	19.7083	19.7080	1.6(-4)
91	62	14,5	-	19.7822	19.7831	2.2(-2)
92	62	18,2	-	19.8742	19.8709	2.5(-3)
93	62	10,8	-	19.9125	19.9112	1.1(-3)
94	60	0,15	-	20.0388	20.0391	1.6(-4)
95	62	6,11	-	20.1658	20.1652	3.6(-4)

**TABLE III:** States of 3:4 System Continued. Notation as in Table I.

State	N	$n_x, n_y$	$E_{TC}$	$E_{QM}$	$E_{AS}$	SD
111	66	2,15	-	21.7467	21.7469	0.5(-4)
112	68	8,11	-	21.8244	21.8237	7.0(-4)
113	70	18,4	-	22.0060	22.0183	3.3(-2)
114	70	14,7	-	22.0939	22.0878	6.0(-3)
115	68	4,14	-	22.1785	22.1784	1.8(-4)
116	70	10,10	22.2606	22.2715	22.2701	1.4(-3)

TABLE III: continued...

117	70	22,1	-	22.2863	22.2819	6.4(-3)
118	72	16,6	-	22.5460	22.5470	4.1(-2)
119	68	0,17	-	22.5631	22.5636	0.2(-4)
120	70	6,13	22.5991	22.6011	22.6006	5.3(-4)
121	72	20,3	-	22.6727	22.6741	8.2(-3)
122	72	12,9	-	22.7355	22.7319	1.9(-3)
123	70	2,16	-	22.9963	22.9966	0.5(-4)
124	72	8,12	-	23.0212	23.0202	8.8(-4)
125	72	24,0	-	23.0398	23.0294	6.8(-4)
126	74	18,5	-	23.0826	23.0609	5.7(-2)
127	74	14,8	-	23.2166	23.2225	5.7(-3)
128	74	22,2	-	23.3197	23.3157	6.3(-3)
129	72	4,15	-	23.4125	23.4124	4.4(-4)
130	74	10,11	23.4325	23.4464	23.4449	1.4(-4)
131	76	20,4	-	23.6122	23.6822	4.9(-2)
132	76	16,7	-	23.7522	23.6834	3.0(-2)
133	74	6,14	-	23.8164	23.8157	2.0(-3)
134	72	0,18	-	23.8252	23.8257	0.2(-4)
135	76	12,10.	23.8654	23.8864	23.8829	3.7(-3)

**TABLE IV:** Highest Quasi-Bound States of the 3:4 System

State <sup>a</sup>	N	$n_x, n_y$	$E_{QM}^b$	$E_{AS}$	SD
142 <sup>e</sup>	78	10,12	24.6151(2)	24.6156	3.5(-3)
143 <sup>e</sup>	76	4,16	24.6454(7)	24.6458	8.8(-4)
144 <sup>e</sup>	80	20,5	24.6463(80)	24.6462	9.3(-2)
145 <sup>e</sup>	78	26,3	24.7924	24.7804	4.8(-3)
146 <sup>e</sup>	80	16,8	24.8373(4)	24.8076	3.2(-2)
147 <sup>e</sup>	80	24,2	25.0086(90)	25.0024	2.2(-2)
148 <sup>e</sup>	78	6,15	25.0268(9)	25.0289	3.9(-3)
149 <sup>e</sup>	80	12,11	25.0366(7)	25.0303	6.3(-3)
150 <sup>e</sup>	76	0,19	25.0873	25.0879	2.0(-5)
151 <sup>e</sup>	82	18,7	25.1540(93)	25.1961	9.2(-2)
152 <sup>e</sup>	82	22,4	25.3709(12)	25.3485	6.6(-2)
153 <sup>e</sup>	80	8,14	25.4053	25.4004	1.5(-3)
137 <sup>o</sup>	77	23,2	24.1684	24.1669	1.1(-2)
138 <sup>o</sup>	75	5,15	24.2273	24.2274	1.6(-3)
139 <sup>o</sup>	77	11,11	24.2429(39)	24.2431	2.0(-3)
140 <sup>o</sup>	79	17,7	24.3909(20)	24.4502	5.6(-2)
141 <sup>o</sup>	79	21,4	24.5691	24.5112	5.7(-2)
142 <sup>o</sup>	77	7,14	24.6171	24.6160	5.1(-3)
143 <sup>o</sup>	75	1,18	24.6662	24.6667	3.0(-5)
144 <sup>o</sup>	79	13,10	24.6849	24.6794	5.8(-3)
145 <sup>o</sup>	79	25,1	24.8559(67)	24.8446	3.0(-2)
146 <sup>o</sup>	81	19,6	24.9061(89)	24.9129	1.1(-1)
147 <sup>o</sup>	79	9,13	25.0041	25.0005	8.5(-3)
148 <sup>o</sup>	77	3,17	25.0686	25.0688	4.6(-3)
149 <sup>o</sup>	81	15,9	25.1151(3)	25.1374	3.3(-2)

**TABLE IV:** continued...

- a. Superscript e/o denotes an even/odd in x state, counted separately for each parity.
- b. The number in brackets gives the last digits different in the smaller diagonalization, e.g. 24.6463(80) stands for 24.6463 in the basis of 1156 even (1122 odd) states and 24.6480 in the smaller basis of 1089 even (1089 odd) states.

**TABLE V:** Some Energy Levels of the 1:2 Hamiltonian

$N^a$	$n_x, n_y$	$E_{MKM}^b$	$E_Q^c$	$E_{AS}^d$	$SD^e$
0	0,0	1.048	1.04778	1.04778	<1.0(-5)
1	1,0	1.744	1.7440	1.7440	1.0(-5)
2	1,0	2.438	2.4387	2.4387	<1.0(-5)
2	2,0	2.439	2.4388	2.4388	4.0(-5)
3	1,1	3.132	3.1297	3.1297	4.0(-5)
3	3,0	3.130	3.1323	3.1323	6.0(-5)
4	2,1	-	3.8192	3.8192	1.2(-4)
4	0,2	-	3.8228	3.8229	1.0(-5)
4	4,0	-	3.8244	3.8244	7.0(-5)
22	10,6	-	15.8079	15.8092	1.2(-2)
22	8,7	-	15.8085	15.8164	1.1(-2)
22	12,5	-	15.8310	15.8218	1.3(-2)
22	6,8	-	15.8376	15.8403	2.4(-3)
22	14,4	-	15.8464	15.8449	4.3(-3)
22	4,9	-	15.8648	15.8646	1.0(-3)
22	16,3	-	15.8722	15.8722	4.1(-3)
22	2,10	-	15.9001	15.9001	2.7(-4)
22	18,2	-	15.9127	15.9129	3.2(-3)
22	0,11	-	15.9458	15.9459	1.0(-5)
22	20,1	-	15.9656	15.9660	2.0(-3)
22	22,0	-	16.0319	16.0317	6.9(-4)

**a.** Principal quantum number  $N = n_x + 2n_y$ .

**b.** Semiclassical results of ref. 26.

**TABLE V:** continued...

- c. Exact quantum eigenvalues calculated in harmonic basis set.
- d. Present AS results.
- e. Standard deviations;  $a(-b)$  stands for  $a \times 10^{-b}$ .

**TABLE VI:** Some "Proper Topology" States of the Henon-Heiles System

$(N, \ell)^a$	$E_y^b$	$E_{\text{SBR}}^c$	$E_{\text{QM}}^d$	$E_{\text{AS}}^e$	$SD^f$
0,0	0.9984	0.9947	0.99859	0.99859	0.6(-5)
1,1	1.9899	1.9862	1.9901	1.9901	3.9(-5)
2,0	2.9560	2.9506	2.9562	2.9562	3.4(-4)
2,2	2.9851	2.9814	2.9853	2.9852	6.0(-5)
3,1	3.9257	3.9225	3.9260	3.9260	4.8(-4)
3,3	3.9837	3.9801	3.9841*	3.9839	1.0(-4)
4,2	4.8986	4.8954	4.8987	4.8987	5.0(-4)
4,4	4.9856	4.9819	4.9863	4.9858	1.0(-4)
7,5	7.831	7.8281	7.8327	7.8316	7.0(-4)
7,7	8.007	8.0038	8.0094	8.0078	2.3(-4)
10,4	-	10.453	10.463	10.457	4.0(-4)
10,10	-	11.040	11.050	11.044	5.0(-4)
11,11	-	12.051	12.065	12.055	8.0(-4)
12,4	-	12.176	12.206	12.180	3.0(-2)
12,6	-	12.296	12.305*	12.296	2.4(-2)
12,8	-	12.477	12.480	12.472	1.9(-2)
12,10	-	12.710	12.712	12.715	3.3(-2)
12,12	-	13.058	13.082*	13.062	6.0(-4)

a. State classification:  $N$ -principal quantum number,  $\ell$ -angular momentum.

b. AS results of Johnson (ref. 7), angular momentum quantized with the Langer correction.

c. AS results of Skodje et al. (ref. 10), EBK quantization of angular momentum.

d. Quantum mechanical results (ref. 39).

**TABLE VI:** continued...

- e. Present AS results quantized with the "modified Langer correction" defined in the text states up to (7,7) average of 10 trajectories, higher states average of 30 trajectories.
- f. Standard deviations.
- \* Average of two quantum mechanically split levels.

**TABLE VII:** Precesor-Type States of the Henon-Heiles System

$(N, \ell)^a$	$E_y^b$	$E_{SBR}^c$	$E_{GST}^d$	$E_{QM}^e$	$E_{ASS}^f$	$SD_S^g$	$E_{ASM}^h$	$SD^k$	$MSD^l$
4,0	4.8698	4.8573	-	4.8702	4.8708	3.6(-3)	4.8708	6.5(-3)	2.9(-4)
5,1	5.8167	5.8167	5.8240	5.8170	5.8168	6.3(-3)	5.8169	1.2(-3)	4.1(-4)
6,0	6.738	6.7077	6.7574	6.7379	6.7341	1.0(-2)	6.7378	2.0(-2)	6.5(-4)
7,1	7.659	7.6556	7.6747	7.6595	7.6527	1.2(-2)	7.6601	2.8(-2)	1.3(-3)
8,0	8.55	8.4919	8.5758	8.5541	8.5353	2.5(-2)	8.5544	4.1(-2)	2.5(-3)
8,2	8.58	8.5965	-	8.5764	8.6018	4.0(-3)	8.5833	3.3(-2)	2.0(-3)
9,1	-	9.4276	9.4593	9.4441	9.4272	3.2(-2)	9.4499	5.8(-2)	5.1(-3)
10,0	-	10.194	10.319	10.305	10.271	5.0(-2)	10.311	8.5(-2)	9.1(-3)
10,2	-	10.358	-	10.318	10.349	1.0(-2)	10.346	7.2(-2)	6.7(-3)
11,1	-	11.127	11.163	11.152	11.131	6.3(-2)	11.174	1.2(-1)	1.4(-2)
12,0	-	11.736	11.956	11.966	11.933	1.0(-1)	11.994	1.5(-1)	2.0(-2)
12,2	-	12.047	-	11.968	12.005	6.7(-2)	12.032	1.3(-1)	1.9(-2)
13,1	-	12.703	12.732	12.762	12.772	1.2(-1)	12.811	2.0(-1)	2.9(-2)
13,3	-	12.914	-	12.890*	12.923	5.9(-2)	12.896	1.5(-1)	4.0(-2)

a. Principal and angular momentum quantum numbers.

b. AS results of Johnson, ref. 7.

c. Skodje et al. (ref. 10) AS results with different  $H_0^F$  (see text).

d. Grozdanov et al. (ref. 13) AS results with another  $H_0^F$  and EBK quantization of  $I_1$ ,  $I_2$  actions.

e. Exact quantum energies (ref. 39).

f.  $E_{ASS}$ , standard AS approach results, switching time  $T = 400$ .

g. Standard deviations.

h.  $E_{ASM}$  modified to minimize separatrix crossing AS results, switching time  $T = 400$ .

k. Standard deviations for  $T = 40$ .

**TABLE VII:** continued...

1. Modified standard deviations (see text).

\* Average of two energies.

**TABLE VIII: Energy Eigenvalue for a Non-Resonant Hamiltonian.**

State	$n_x, n_y$	FT <sup>a</sup>	$E_{12}$ <sup>b</sup>	$E_{12P}$ <sup>c</sup>	$E_{16}$ <sup>d</sup>	$E_{16}$ <sup>e</sup>	$E_{QM}$ <sup>f</sup>	$E_{AS}$ <sup>g</sup>	SD
36	10,0	7.7419	7.7420	7.7418	-	-	7.7423	7.7419	4.3(-5)
37	1,5	7.8996	7.8999	7.8999	-	-	7.8996	7.9000	8.9(-5)
38	3,4	7.9522	7.9529	7.9527	-	-	7.9525	7.9528	8.3(-5)
39	5,3	8.0256	8.0264	8.0260	-	-	8.0259	8.0261	6.0(-5)
40	7,2	8.1213	8.1225	8.1220	-	-	8.1220	8.1221	8.0(-5)
41	9,1	8.2428	8.2438	8.2432	-	-	8.2435	8.2433	5.2(-5)
42	11,0	8.3924	8.3936	8.3932	-	-	8.3939	8.3932	1.0(-4)
74	4,6	-	10.8726	10.8676	10.8696	10.8618	10.8657	10.8667	2.4(-3)
75	6,5	-	10.9149	10.9071	10.9103	10.9013	10.9053	10.9061	4.5(-4)
76	15,0	-	10.9485	10.9431	10.9455	10.9379	10.9439	10.9408	5.6(-4)
77	8,4	-	10.9816	10.9717	10.9756	10.9658	10.9700	10.9705	5.1(-4)
78	10,3	-	11.0761	11.0641	11.0689	11.0584	11.0612	11.0624	1.8(-3)
79	12,2	-	12.2024	11.1876	11.1942	11.1836	11.1856	11.1883	8.2(-3)
80	14,1	-	11.3656	11.3493	11.3575	11.3474	11.3484	11.3434	1.2(-2)
81	1,8	-	11.4233	11.4218	11.4222	11.4153	11.4129	11.4190 <sup>r</sup>	4.1(-3)
82	3,7	-	11.4238	11.4186	11.4206	11.4124	11.4158	11.4129 <sup>r</sup>	9.5(-3)
83	5,6	-	11.4447	11.4341	11.4390	11.4294	11.4325	11.4303	5.2(-3)
84	7,5	-	11.4885	11.4737	11.4890	11.4694	11.4713	11.4713 <sup>h</sup>	1.4(-3)
85	16,0	-	11.5729	11.5633	-	-	11.5324	11.5519 <sup>h</sup>	1.8(-3)

**a.** SC results by FFT method (ref. 42).

**b.** SC quantization of 12th order BGNF (ref. 4a).

**c.** SC quantization of 12th order BGNF with Pade resummation (ref. 4a).

**d.** SC quantization of 16th order BGNF (ref. 4b).

**e.** SC quantization of 16th order BGNF with Weyl quantization rule (ref. 4b).

**TABLE VIII:** continued...

- f.** Exact quantum-mechanical values (from ref. 41).
- g.** Present AS results, average of 25 trajectories with switching time  $T = 400$ .
- h.** Levels above classical escape energy  $E = 11.4601$ .
- r.** Quantizing trajectories in 1:2 resonance zone (ref. 13).

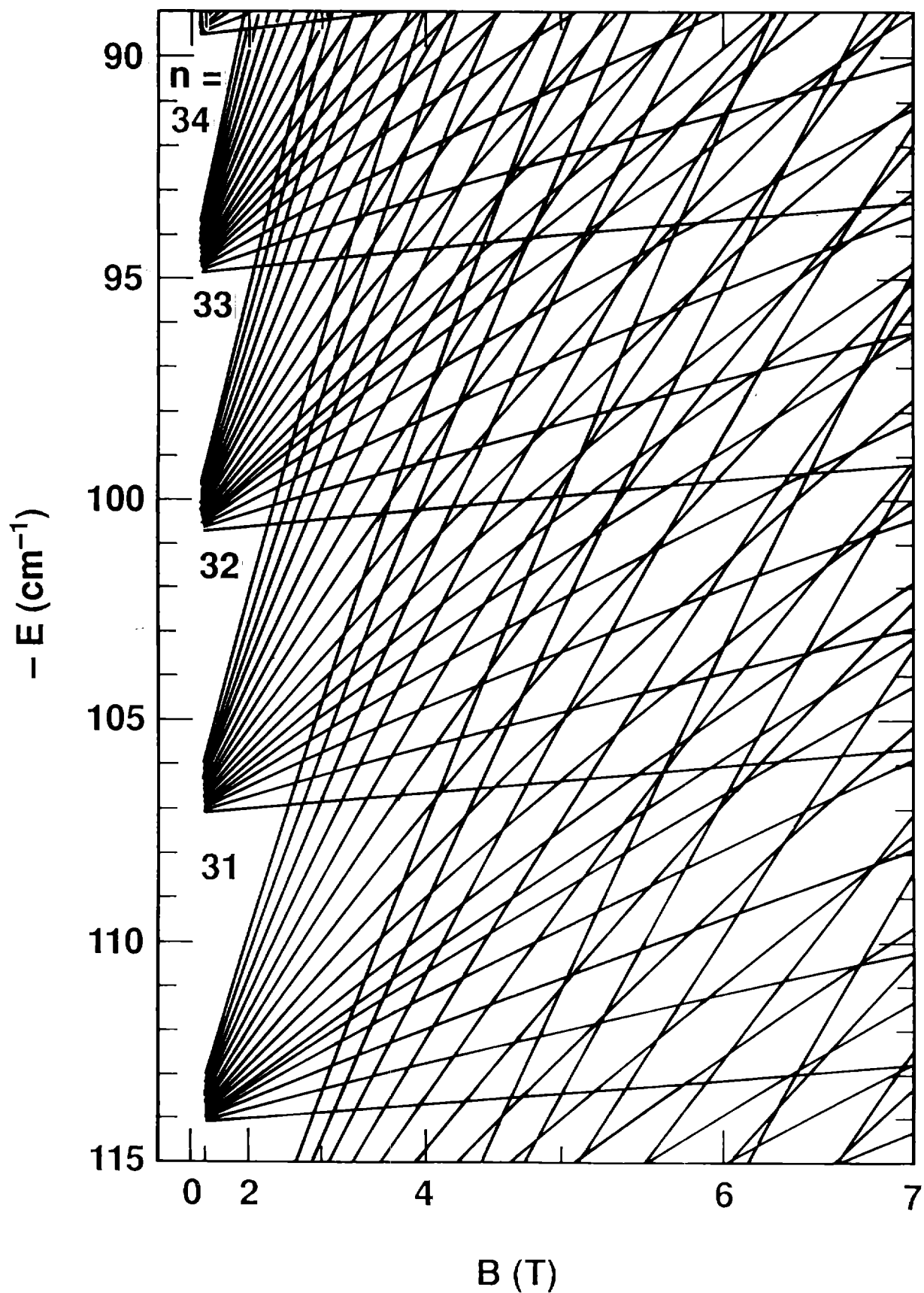


Figure 1

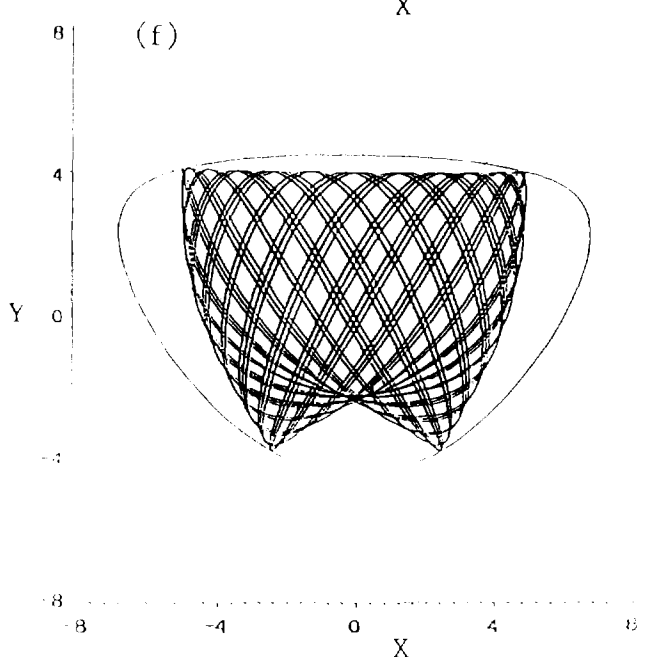
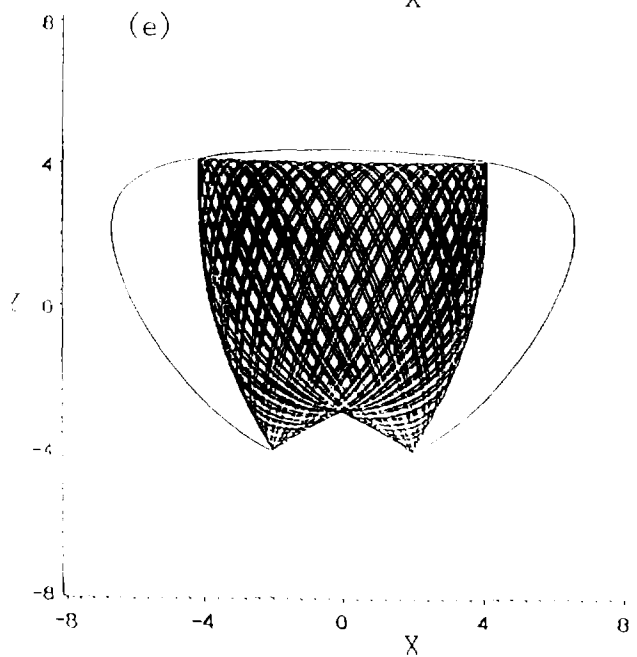
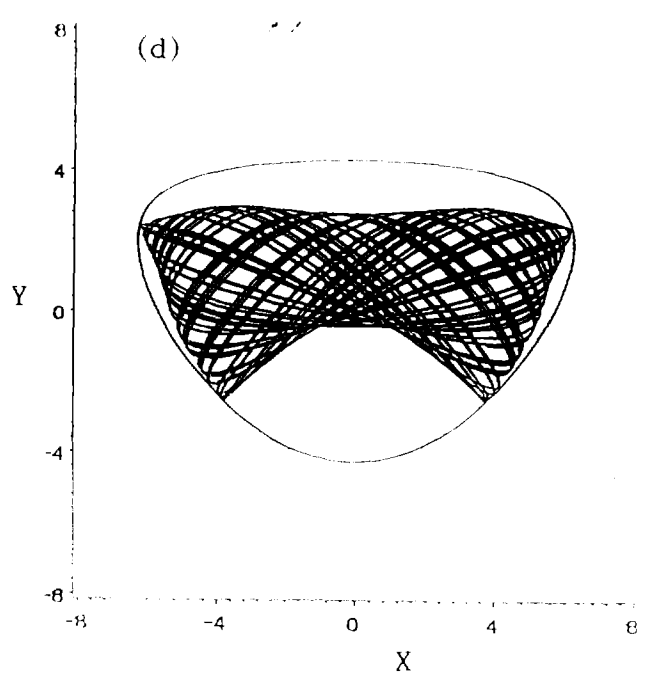
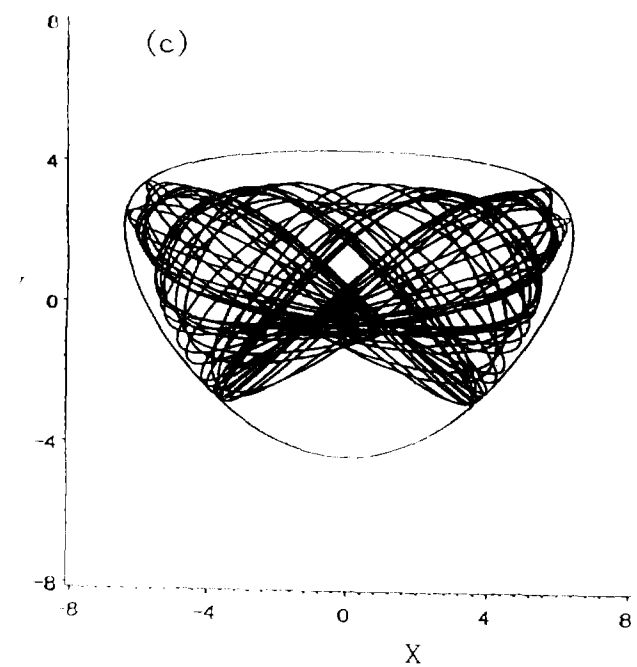
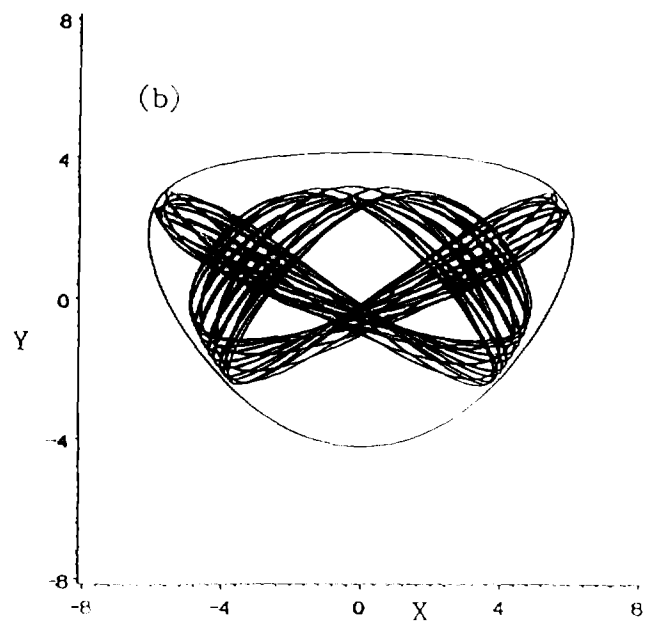
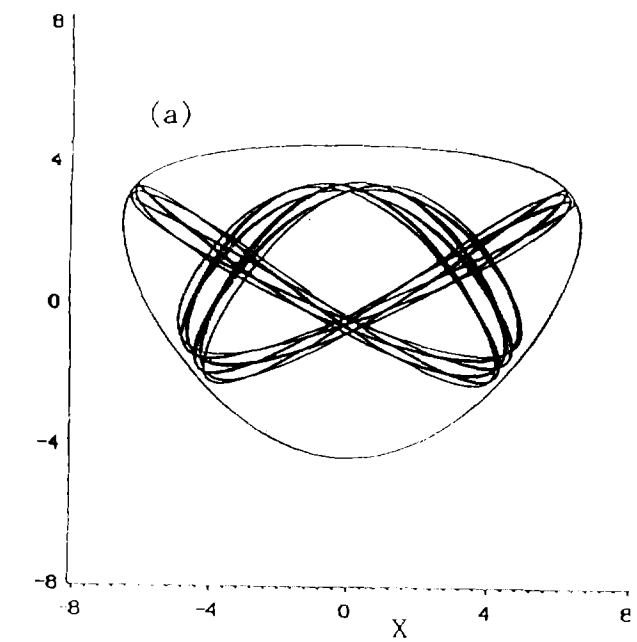


Fig. 2

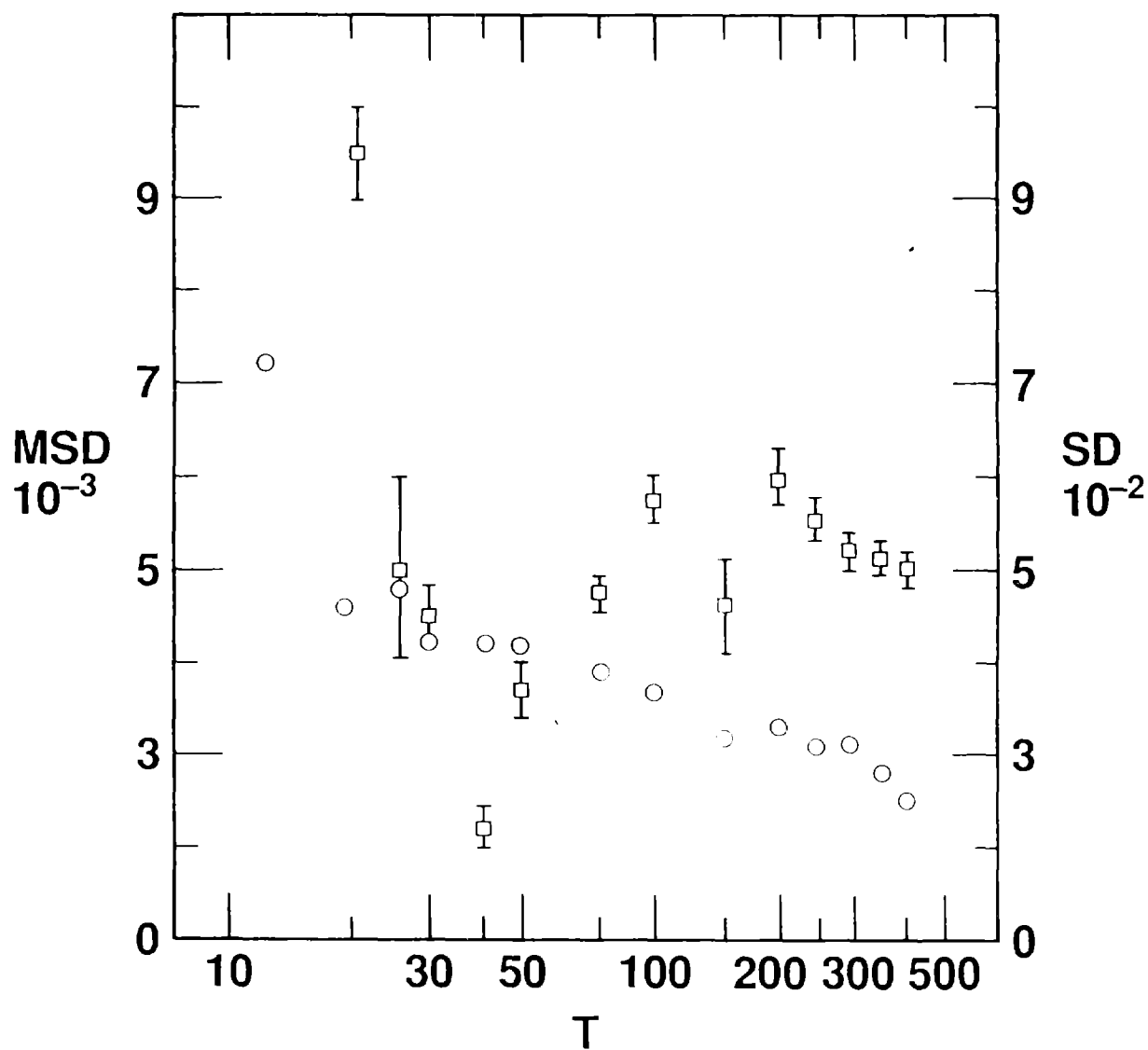


Figure 3

